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United States
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ARS-81

June 1990

Proceedings of the International Symposium on Water Quality Modeling of Agricultural Non-Point Sources, Part 1

June 19-23, 1988
Utah State University
Logan, Utah

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The papers presented in this proceedings are in two groups: invited manuscripts on specific topics and poster presentations. The invited papers, which make up the bulk of the papers published here, were treated as technical journal papers and received peer and extensive editorial review. The contributed poster papers received editorial review.

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Proceedings of the International Symposium on Water Quality Modeling of Agricultural Non-Point Sources, Part 1

June 19-23, 1988
Utah State University
Logan, Utah

Donn G. DeCoursey, Editor

Sponsored by:
International Science and Education Council
Office of International Cooperation and Development, USDA
Agricultural Research Institute
Agricultural Research Service, USDA
Forest Service, USDA
National Agricultural Chemicals Association
National Association of State Universities and Land-Grant
Colleges
Soil Conservation Service, USDA
Utah Agricultural Experiment Station
Utah Water Research Laboratory

PREFACE

An International Symposium on Water Quality Modeling of Agricultural Non-point Sources, was held at Utah State University, Logan, Utah, June 19-23, 1988. The purpose of the symposium was to foster international discussion and present the state-of-the-art in water quality model development and use. The symposium was sponsored by the International Science and Education Council (ISEC) and organized by the Scientific and Technical Cooperation Division (STC) of the U.S. Department of Agriculture (USDA), Office of International Cooperation and Development (OICD). In addition to ISEC and OICD, cosponsors included the Agricultural Research Institute; Agricultural Research Service, USDA; Forest Service, USDA; National Agricultural Chemicals Association; National Association of State Universities and Land-Grant Colleges; Soil Conservation Service, USDA; Utah Agricultural Experiment Station and Utah Water Research Laboratory.

The symposium welcome was given by Provost, Peter Wagner, representing Utah State University President, Stanford Cazier. Dr. Paul Larsen, Vice-President for extension, introduced H. Rouse Caffey, Chancellor, Louisiana State University, Agricultural Center and Co-Chair of ISEC, who gave the opening address. Howard S. Marks, Associate Administrator of OICD, introduced Deputy Secretary of Agriculture, Peter C. Myers, who presented the challenge to symposium attendees.

The quality of surface and subsurface water is a major problem that will increase in importance in the years ahead. The computer model is a powerful tool in assessing the magnitude of the problem and in determining optimal management strategies. Many models are available and many more will be developed. In recent years numerous symposia have provided descriptions and models of the physical, biological, and chemical processes that determine water quality. However, many of these models have not been used because of a lack of user-level information, and a lack of communication between decision-makers (users) and modelers. This symposium serves to initiate better communication between these two groups.

Invited speakers from academia, industry and government were selected to present the state-of-the-art from both the model developer's and user's perspectives. Most authors provided pre-symposium drafts of their manuscripts which were distributed to participants. Two brief 15 minute presentations on each subject were made: one from the U.S. and one from another country. The presentations were followed by 40 minutes of discussion. This format was provided as a forum to obtain maximum interaction between scientists from different countries and between model developers and model users. Three keynote papers (putting water quality into perspective, health issues, and socio-economic and political issues) were assigned and presented during the symposium. The invited speakers presented state-of-the-art reviews of modeling on the following topics related to agricultural non-point sources:

- i) leaching models (modeler's and user's perspective)
- ii) sediment yield/surface runoff models (modeler's and user's perspective)
- iii) groundwater models (modeler's and user's perspective)
- iv) surface water models (modeler's and user's perspective)
- v) integrated models (modeler's and user's perspective)
- vi) spatial variability and scale
- vii) prediction/comparison - simple/complex
- ix) risk analysis/confidence limits
- x) software engineering
- xi) parameter identification
- xii) data base development.

In addition to invited speakers on the above subjects attendees were given the opportunity to present poster papers on their modeling efforts and write extended abstracts of their material.

These proceedings include the peer reviewed and edited papers presented by the invited state-of-the-art speakers, a transcript of the discussions following presentations of each pair of papers, the presentations of the keynoters, and extended abstracts describing poster presentations. These papers are excellent references to the subjects presented and include extensive bibliographies. They provide a state-of-the-art description of model development. Recommendations for improvement in both model content and user interaction are expressed very well throughout the papers and discussions.

The Steering Committee for the symposium consisted of Donn G. DeCoursey, Research Leader, Agricultural Research Service, Chairman; Martha B. Steinbock, USDA, OICD, Executive Secretary; Stan Cath, Executive Director, Agricultural Research Institute; Thomas J. Gilding, National Agricultural Chemicals Association; and Norman R. Scott, Director, Cornell Agricultural Experiment Station. The committee wishes to thank Dr. Paul Larsen and the staff at Utah State University for providing session chairpersons and discussion transcribers, and for the excellent facilities and warm welcome. We also want to thank the individuals who gave their time to provide the in-depth reviews of all the invited papers and keynote addresses. We especially want to thank Mrs. Virginia Ferreira who did such an excellent job editing all of the papers. Finally, we wish to thank all the authors and attendees for the excellent papers and discussions.

Donn G. DeCoursey
Editor

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Opening Session

INTERNATIONAL SYMPOSIUM ON WATER QUALITY MODELING OF NONPOINT AGRICULTURAL SOURCES - OPENING REMARKS.

H. Rouse Caffey¹

Thank you, Dr. Wagner, for your opening remarks, and Dr. Larsen for your introduction. It is a great pleasure to be here today to open this international symposium on water-quality modeling of agricultural nonpoint sources.

On behalf of the International Science and Educational Council (ISEC) and the co-sponsors of the symposium, I would like to welcome all of you to Logan, and some of you, to the United States.

ISEC is a forum where representatives of U.S. Universities and USDA work together to coordinate, plan and mobilize resources to carry out international activities. The council also makes policy recommendations to the Secretary of Agriculture, and the presidents of the National Association of State Universities and Land Grant Colleges and the American Association of State Colleges and Universities.

As part of its mission, ISEC began several years ago to sponsor, along with the USDA Office of International Cooperation and Development, one or two international symposia each year to focus international attention on issues important to world agriculture. The first such symposium, held in April 1987 at Ohio State University, dealt with Africanized bees and bee mites.

We could not be considering a more important topic here today than water quality. Two years ago the ISEC council was asked to help select a topic for the 1988 symposium. Although several excellent proposals were put forward, in the council's judgement the need for water quality research was emerging as the central issue for the late 1980's.

Our judgement was correct. For 1989 the U.S. Joint Council on Food and Agricultural Sciences reported to the U.S. Secretary of Agriculture that maintaining and preserving water quality should be the top priority for the United States Agricultural Research Community. According to the joint council, "Providing a long-term water supply of acceptable quality in the presence of sustained agricultural, industrial, municipal and recreational activities continues to be a challenge. A better understanding of...the environmental fate of chemicals (persistence, mobility, transformation and degradation in the soil and water systems) is essential to prevent inadvertent contamination of water sources."

Of course, agriculturally-related water quality research is needed, not only in the United States, but also in all the nations of the world where agricultural production increasingly is affecting the environment. Thus this forum for international dialogue is both appropriate and timely in addressing a national, as well as an international need.

It is our challenge here this week to move forward in developing the important tool of water models to help meet this need. And I am confident that we will be successful, to the betterment of the world agricultural community, and to the general public in all our nations.

¹H. Rouse Caffey, Chancellor, Louisiana State University, Agricultural Center (ISEC Co-Chair), Baton Rouge, Louisiana.

Before turning the platform over to Dr. Larsen, I would like to thank the agencies and individuals who worked for the last two years to bring us together here this week:

- (1) The Office of International Cooperation and Development for providing international coordination, staff support, and financial resources;
- (2) The Agricultural Research Service, in particular Dr. Donn DeCoursey, who served as chairman of the steering committee, for overall planning, program selection and financial support;
- (3) The USDA Soil Conservation Service, the Forest Service and the National Agricultural Chemicals Association for financial support;
- (4) The Agricultural Research Institute for their assistance in financial and program planning; and of course,
- (5) Utah State University for providing moderators, rapporteurs, and these beautiful facilities.

And thanks to you all for making the efforts to be here. As a testimony to the importance of this endeavor, we have approximately 150 experts here this week representing federal, state, and private sector organizations in 15 countries and over 30 states. I wish you every success in the task before you.

SYMPOSIUM CHALLENGE FROM DEPUTY SECRETARY OF AGRICULTURE - INTRODUCTORY COMMENTS

Howard S. Marks¹

Good afternoon ladies and gentlemen. I am Howard Marks, Associate Administrator of USDA's Office of International Cooperation and Development or OICD as we are known. OICD manages the international programs of USDA not specifically related to trade issues.

I am pleased to have this opportunity to participate in the international science and educational council's and U.S. Department of Agriculture's International Symposium on Water Quality Modeling of Agricultural Non-Point Sources.

I want to thank all of the department's agencies and private cooperators for the time, energy, and resources that have been devoted to make the symposium a success. Each and every one of your staff deserves to be commended for their hard work. It is also appropriate to recognize the input of our hosts -- Utah State University in providing such a beautiful setting for this International Symposium.

The topic we are here to discuss is water quality. The international viewpoints that will be expressed over the next three days will serve to highlight why USDA's joint council for food and agricultural sciences has made the improvement of water quality its top priority.

International cooperation is especially significant when addressing water quality issues because water transcends national boundaries. Problems in one country can potentially affect the water supply in neighboring countries. By sharing knowledge, results, and experiences, nations can save time and money by avoiding the duplication of research. Each country can adapt international research results for application to its specific water quality issues.

I am pleased to have the honor to introduce our featured speaker today.

INTRODUCTION OF DEPUTY SECRETARY OF AGRICULTURE, PETER C. MYERS

Mr. Myers was appointed Deputy Secretary just over two years ago in June 1986. In that role he assists Secretary Richard Lyng in supervising all activities of the department.

Before entering the government, Mr. Myers operated his own row crop and livestock farm in Missouri. During this period he was active in the state's Pork Producer's Association, Cattlemen's Association and served on the Board of the Missouri Farm Bureau Federation.

Before assuming his duties as Deputy Secretary, Mr. Myer's served as Assistant Secretary for Natural Resources and Environment, and Chief of the Soil Conservation Service.

As you know, the Soil Conservation Service develops and carries out our nation's soil and water conservation program. With the help of its cooperators, the SCS inventories and assesses soil, water, and plant resources. It also plans and applies conservation practices to reduce soil erosion as well as maintain the land's productivity.

Because of his broad-based experience in agriculture and special expertise in soil and water issues, it is my pleasure and honor to welcome Deputy Secretary of Agriculture, Peter C. Myers, to Logan, Utah.

¹Howard S. Marks, Associate Administrator, Office of International Cooperation and Development, Utah State University, Logan, Utah.

SYMPOSIUM CHALLENGE FROM DEPUTY SECRETARY OF AGRICULTURE

Peter C. Myers¹

MODELING FOR THE REAL WORLD

When Abraham Lincoln created the United States Department of Agriculture back in 1862, he called it "the people's department." One reason that USDA agencies are so deeply involved in water quality issues today -- 126 years later -- is that water quality problems are people problems.

People help cause water pollution. People are affected by water pollution. And people can do something about water pollution.

Our special concern at this symposium is the pollution of water by agricultural chemicals and agricultural activities. By and large, this means nonpoint source water pollution. Point source problems generally occur off the farm and so are outside the scope of this symposium. (An exception would be feedlot runoff.) Therefore, prevention of nonpoint pollution offers at best only a partial solution to the total water quality problem. But it is nevertheless an important goal and one that rightly concerns all of us here today.

Reducing nonpoint pollution is a legitimate aim of government at all levels, of university research and extension, and of industry. It represents a significant challenge both here in the United States and abroad. It is gratifying, therefore, to see that the entire spectrum of nonpoint concerns will be addressed at this symposium, and that the Office of International Cooperation and Development, working with their governmental and private cosponsors, have succeeded in gathering such a distinguished group of international experts. By meeting together face-to-face, I am confident we will learn a great deal from one another, and benefit people in all countries.

We have two main purposes for being here. Our first purpose is immediate: Improving communications among the designers and the users of models, including professionals in the different countries represented here. During this week and after we go home, we should make a major effort to improve our network for exchanging technical information. Modelers and model users should explore and capitalize on opportunities for working more effectively together.

Our second purpose is broader and longer term: To maintain and improve water quality.

There is an old story that puts this second purpose into some perspective. It concerns a man who came across three other men working in a rock quarry. When he asked them what they were doing, the first replied, "I'm making my living." The second man said, "I'm cutting stone." But the third said, "I'm helping build a great cathedral."

I hope that everyone at this symposium will take the broad view that the third man took. The ultimate goal for building water quality models is not to have bigger and better models. We should not be building them merely to develop a better understanding of the dynamics of soil and water chemistry -- even though that perhaps should be an important secondary goal. Our primary purpose must be to help find ways -- economically viable ways -- for the farmers in our respective nations to avoid polluting surface and ground water.

¹Peter C. Myers, Deputy Secretary, U.S. Department of Agriculture.

We need models that are useful on the farm. Models that will give us good answers quickly. Decision models for specific aspects of agricultural operations. Models that Soil Conservation Service conservationists and technicians and Extension agents can use as they advise farmers on conservation practices, land treatment, and farming practices, including chemical management. Models that farmers themselves can eventually use to select the most appropriate management techniques.

Models have enormous potential as aids in making on-the-spot decisions about resource management practices that are environmentally safe and economically sound. I hope we agree that this should be the major purpose of water quality modeling. Beyond this, however, models do serve three other very important functions.

First, models identify critical gaps in fundamental knowledge. Modeling may be defined as the integration of existing knowledge into a logical framework. As we attempt to assemble the facts we know, we can more clearly see what we do not know. Then we can do the research needed to fill these gaps.

Second, models provide guidelines for getting the most out of our experimental research. Once we have filled the critical gaps in our knowledge base, models can help us zero in on the best experimental approaches to solving the problem. We can ask the "what if" questions, and in a well-designed model the answers will be good preliminary indicators of what really will happen under experimental conditions. In this respect, models make us much more efficient. They save us time and money, and they enable us to pursue those lines of inquiry most likely to be successful.

And third, models help us set priorities. Once a model is operational, it lets us broaden our focus. It tells us not only what is likely to happen under existing conditions, but also what is likely to happen when certain variables are changed. By giving us this broader and longer term perspective, it can help us decide how best to change farming practices to improve the quality of water. It may also help us minimize the adverse effects on water quality of droughts, heavy rains, floods, insect plagues, and other extreme events.

Currently, a major limitation to progress through modeling is the diversity of soils, crops, climates, topographies, management scenarios, and chemicals that must be considered. For example, SCS has classified the soils in this country into more than 15,000 distinct soil series. To be most effective and accurate, your models must simulate all the natural processes in the root zone, in the underlying formations, and in streams, lakes, and ground water. They must also simulate the cultural practices that affect those processes.

Sophisticated computer models, therefore, will have to draw upon our knowledge in many areas of science -- soils, geology, hydrology, toxicology, meteorology, microbiology, chemistry, and other fields. Synthetic farm chemicals are both more difficult and more costly to measure than are bacteria and dissolved solids. Modelers must also take into account the EPA guidelines on safe levels of various compounds. Should we also look at the least-risk aspect in models? Your task, undeniably, is incredibly complicated, and I can certainly appreciate how difficult it is.

Yet I stand before you today to say that we need those models, and we need them soon.

The Agricultural Research Service has already done a great deal of work in developing and refining models for water quality and other areas. ARS, as most of you probably know, is USDA's principal scientific research agency and is very active in water quality research.

ARS scientists have developed a number of models that simulate the movement of water and associated materials over and through the soil:

- * One of these is called the Erosion Productivity Impact Calculator -- EPIC, for short. It estimates erosion damages.
- * The Root Zone Water Quality Model is in a preliminary stage of development, and I understand that the first version of this model is on display at the symposium.
- * Another is a model called CREAMS, which is short for Chemicals Runoff and Erosion from Agricultural Management Systems. CREAMS estimates the effects of runoff and erosion on surface water quality.
- * A model called GLEAMS, Groundwater Loading Effects of Agricultural Management Systems, is a modification of CREAMS for estimating rates of chemical loading in groundwater.

Several other water quality models are now in use or development.

Modeling of groundwater quality is a key part of ARS's highest research priority for 1988 -- improving the quality of groundwater. This also is the highest priority on this year's needs list of USDA's Joint Council for Food and Agricultural Sciences. So it is appropriate for me to quickly highlight ARS's new Strategic Groundwater Plan. This plan is hot off the press. It is printed in a series of three booklets which cover the most serious groundwater pollutants associated with agricultural activity -- pesticides, nitrates, salts, and toxic trace elements.

The plan documents the more pressing research objectives and tasks in a logical, systematic way. It recognizes that limitations on funding must be factored into the research. Therefore, the plan concentrates on those things we can afford to do. Among our objectives in releasing the plan are to bring these needs to the attention of the entire scientific community and to encourage others to become involved.

Among the many other projects that ARS scientists are working on are several that I expect will have a decidedly positive impact on water quality:

- * Using biological pest controls as non-chemical alternatives or complements to synthetic pesticides.
- * Improving ways of applying pesticides, including controlled release through starch encapsulation to reduce total pesticide use and improve pesticide targeting.
- * Developing more efficient irrigation methods to reduce such problems as salinization and excessive infiltration of water and agricultural chemicals below the root zone.
- * Breaking down pesticide residues using genetically engineered organisms.

This is the real world of research, and the technology is already moving onto the farm. Is the technology also moving into the models?

Most scientists tend to be conservative about releasing models that do not incorporate the concepts and processes that they consider critical to the simulation of real-world phenomena. For example, ARS scientists are among many looking at a process called preferential flow -- meaning the rapid movement of water through earthworm holes, root channels, and natural soil fissures. Preferential flow is thought to play a key role in chemical movement.

I also understand that we haven't been able to characterize preferential flow well enough to allow its incorporation into models. Do we know what preferential flow means in terms of human health and environmental safety? While processes such as preferential flow may deserve additional attention in model development and water quality research, the time available for model improvement is limited.

Those of us facing the political realities of a concerned community can't wait for perfect models. We need to put what we know now into practice. Even though existing models need further refinement, they can and should be used in selecting and evaluating solutions to specific problems. This would pay immediate dividends in the form of better management decisions. It would also give you some real-life data for further improvements in the performance and reliability of your models.

USDA agencies are already gearing up to do what they can with what they know. SCS and the Extension Service, for example, have already developed a memorandum of understanding on how to address problems associated with agricultural use of chemicals.

Farmers are moving ahead, too. Many farmers have their own computers. Inevitably, farmers are going to use those computers to help them select appropriate farm management systems. Many already use simple nutrient management models.

Given the diversity of users, it is imperative that practical water quality models for use not just by scientists, not just by government field workers, but eventually by farmers as well. I'm talking about user-friendly models that run on personal computers, or at least that can be easily and cheaply accessed by PC's.

I'm also talking about models that take into account the economics of farming. We can't forget that farmers are in business. And if they don't make a profit, they can't afford to protect the environment.

Models clearly show promise as bright new tools to help all of us do a better job. But in our enthusiasm about the benefits of modeling, we ought to remember that models by themselves are not going to solve our problems. Let me suggest a few warnings about models and their ultimate utility.

First, the major assumptions in the model must conform to known and accepted scientific facts; otherwise, the model that we construct will be neither objective nor scientifically defensible.

Second, model design must be flexible enough to accommodate new data and knowledge. For example, as we move toward greater use of slow-release pesticides and fertilizers, the model must be able to take into account our expanding knowledge and use of these methods.

Third, solutions identified by the model must be confirmed by experiment. The model should be viewed as an aid for decision-makers, not as a finely-tuned simulator of real-world conditions. Because there are so many uncertainties in the parameters that characterize soils, climates, landscapes, and chemicals, the predictions of most models are estimates -- highly educated guesses, if you will -- and as such are no substitute for onsite measurements and data analyses.

And finally, the model must never become an end in itself. I have little use for research for its own sake. Models, like any other research tool, are useful only when they contribute to solutions of real problems.

By working together, we can build that great cathedral and move toward solutions of the water quality problems facing our world.

PUTTING WATER QUALITY INTO PERSPECTIVE QUALITY VERSUS QUANTITY

R. Gras¹

ABSTRACT

INTRODUCTION

Water quality of surface waters - rivers, and lakes - changes greatly from season to season and even fluctuates during a given day. The changes reflect natural cycles of river discharges, meteorological conditions, and simple daily fluctuations in solar radiation which affect water biology. Groundwater quality also changes, but not as quickly. In addition to natural causes, water quality changes reflect the consequences of abstraction for water supply, the evolution of agricultural practices and urban and industrial waste inputs as well as the success of wastewater treatment programs.

What is surprising is that water resources management once focused only on quantity. Quality concerns were often considered secondary objectives. This is often true even today. Is this emphasis reflecting the fact that questions relating to water quality were not always felt as acutely in the past as today in developed countries due to growing surface and groundwater pollution in the recent decades? Or could it be that consequences of developments on water quality are not always immediately perceptible. Emphasis on water quantity is somewhat understandable; in countries where water resources are scarce, efforts were first toward making the best use of resources in terms of quantity. However, it is reasonable to think that the more scarce the resource, the more attention should be paid to protect it. The problem is that it is not obvious that projects, mostly oriented toward electricity generation, irrigation, and navigation may have potentially impaired water quality. So, if planning has stated that the goal is to increase water resources for those types of uses, no one will really care much about water quality.

Water quality should be taken into consideration in any project, and it is short-sighted to restrict the problem of water resources management to quantitative aspects. We cannot talk about water quality without having one or more specific objectives in mind. Furthermore, the water resource cannot be examined in terms of quality without knowing how the resource is to be used. Knowing the uses of concern, criteria can be defined enabling the water quality to be apprehended. A shoe of good quality means nothing if you don't precisely state the purpose for which you intend to use it. For example, the most comfortable and tough boot imaginable cannot be considered a good quality ballet slipper.

Having defined the use of concern, and having defined the parameters and criteria to consider, it is still necessary to examine other elements, to ensure proper water quality decisions are made.

THE RELATIONSHIP BETWEEN WATER QUANTITY AND QUALITY

Let us first assume that water quality could be measured in terms of some parameter value, for example temperature. What is the meaning of a 21°C reading for a water body? Is it warm? Is it cold? The same temperature does not have the same significance for a mountain creek as for a large stream, for a river in the north of Canada as for a river of central India. So climate, and

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season as well, must be considered when judging the meaning of the temperature. A temperature of 21°C may be extremely warm for water in winter and rather cold for water in summer. Even during the same day and within the same water body, 21°C could be considered warm or cold depending on where it is measured. For example, water measured in the deep layers of a stratified lake should be colder than water measured at the very surface. Fish temperature requirements also vary with season and physiological factors: spawning for brown trout requires temperature around 10°C, but adult trout grow faster at 16 or 18°C.

Generally it is clear that a set of data for water quality could only become completely significant if peripheral considerations are accounted for. One of those considerations is related to quantitative aspects of the water resource.

If dissolved or solid loads in rivers come from external inputs, it should be reasonable to expect that an increase in river discharge is likely to reduce concentrations by dilution. This should be the case of fairly constant sources of load inputs like those from sewage effluents from urban or industrial origin.

For example, table 1 shows the results of statistical analysis of a data set of Rhine water quality parameters collected by the International Commission for the Protection of the Rhine against Pollution during the period 1959-1974. It is very clear that low BOD values are associated with high discharges and high (BOD) values with lower discharges. Is this observation an illustration of dilution? Table 2 shows the same type of statistical analysis as table 1, this time not with concentration values but with "pollutant" loads. If dilution is the only process at work, load values should not be organized according to discharge but should remain practically constant. It appears, in fact, that high BOD values are associated with high discharges and low BOD values with low discharges.

More than BOD, phosphate contents of suspended solids could be assumed to be representative of domestic sewage inputs in a river. For a river like the Rhine in its middle reaches, the total upstream input could be considered fairly constant. The curve representing the relation between phosphate contents of suspended solids and discharge (fig. 1) looks like a hyperbolic function, indicative of a constant load. Nevertheless, looking in more detail, it appears that the load is slightly higher for high discharges than for low discharges. This means that in addition to dilution processes, other processes should be taken into consideration.

Hydraulics tells us that, in the subcritical flows that usually occur in a river, water particles have a lower velocity than those of a wave; therefore, when discharge increases due to a heavy rain upstream, at the beginning of the period of increasing flow the water flowing in the middle or lower stretches of a river is of local origin. It is only some time later that runoff from the catchment area reaches the lower section of the river.

Hydrology helps interpret the data by telling us that discharge response to rainfall consists in a rapid increase of flow, then a more-or-less rapid decrease, followed by a slow exponential decrease leading back to the dry season base flow. Each period corresponds to a different source of water feeding the river. The first stage is mainly runoff water associated with the suspended solid load due to soil erosion. The second stage consists of a mixing of runoff and interflow, both flows having different water qualities. Interflow cannot transport substantial solid loads but has a dissolved load due to the relatively short distance of travel of water particles in the ground. The final stage consists mainly of ground water flow - water which has a higher dissolved load due to the generally long residence time in the ground.

We have not yet found an answer to the problem that an increase in discharge usually leads to an increase in river load. This is particularly visible with suspended material. Nearly all rivers carry high suspended material loads during high flow or flood. According to Huber Hellmann (1987),

Table 1.
Main groups of parameter values of Rhine water quality expressed
in concentrations at Braubach based on International Commission of
the Rhine data collected from 1959 to 1974, from Sabaton (1983).

Concentration								
Group	Season	Discharge	DO	BOD	NH4	NO3	KMNO4	pH
43	Winter	High	Very High	Low	Fairly low	Mean	Low	Mean
46	Fall Spring	Very High	High	Low	Low	Mean	Low	Mean
22	Summer	High	Mean	Low	Very Low	Low	Low	High
26	Summer	Mean	Mean	Mean	Low	Low	Low	Fairly High
33	Summer	High	Mean	Mean	Low	Mean	Low	Mean
23	Summer	Fairly Low	Low	High	High	Low	High	Fairly Low
9	Winter	Mean	Mean	Fairly High	High	Very High	Mean	Low
10	Winter Spring	Low	Mean	High	Very High	Very High	Mean	Low
12	Spring Fall	Very Low	Very Low	Very High	Very High	Low	Very High	Very Low
15	Winter	Low	Fairly High	High	High	Mean	High	Low
48	Winter	Mean	High	High	Mean	Very High	Mean	Mean
29	Summer	Mean	Low	Mean	Mean	Mean	Mean	Mean

this very common observation should "astonish those who regard the visible dirt in flowing waters mainly as a consequence of industrial development. Were this so, then an increase in discharge would bring about a dilution of the inevitable contamination and the suspended solids content would become smaller". Although this comment needs to be considered with some restrictions, effects of land use on suspended solids content have to be observed. Think about the drastic change in urban areas. Acute surface water pollution comes from urban changes in drainage conditions and associated processes during storm events. It remains true however, that the highest suspended solids loads occur in natural rivers during the flood or high discharges periods.

Suspended solids content of a river is the result of several specific processes; soil erosion and wash-out, river bed and bank erosion, and sedimentation of suspended solids in areas of low water velocities or during falling discharge periods. All these processes result in a suspended solid content relationship with discharge in the form of figure 2. This shows different values of

Table 2.
Main groups of parameter values of Rhine water quality expressed
in loads at Braubach (same reference as table 1).

← Load →								
Group	Season	Discharge	DO	BOD	NH4	NO3	KMNO4	pH
16	Winter Fall	Very High	Very High	Very High	Very High	Very High	Very High	Mean
9	Any Season	High	High	Mean	Mean	High	High	Mean
8	Any Season	High	High	Mean	Mean	High	High	Mean
7	Summer	Mean	Mean	Mean	Low	Mean	Mean	Mean
3	Spring Summer	Mean	Mean	Low	Low	Low	Mean	Mean
4	Spring Fall	Low	Low	Low	Low	Low	Fairly Low	Mean
5	Spring Fall	Very Low	Very Low	Very Low	Very Low	Very Low	Very Low	Mean
1	Winter Fall	Very Low	Very Low	Low	Mean	Low	Very Low	Low

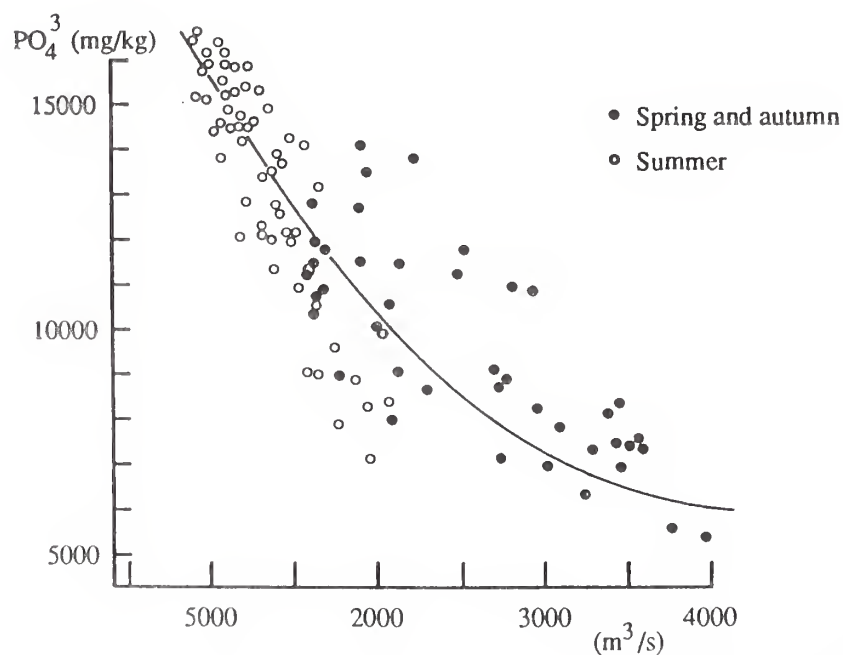


Figure 1.
Phosphate contents of suspended solids in the Rhine as a function
of discharge at Hoblenz in 1974 (after H. Hellmann 1987).

suspended material for the same discharge depending on its evolution with time: higher values for rising discharges and lower values for falling discharges. The mean curve could be represented by a power function such as:

$$S = a Q^b \quad [1]$$

where S = mass of suspended solids [M],
 Q = discharge [$L^3 T^{-1}$], and
 a, b = parameters.

To represent the pear shape, however, it is necessary to introduce time variation of discharge. One example is a stochastic model such as proposed by Duong for the Mississippi:

$$S_t = C_1 Q_{t-1} + C_2 Q_{t-2} + d_1 S_{t-1} + d_2 S_{t-2} + V_t \quad [2]$$

where S = sediment discharge,
 Q = water discharge,
 V = noise term,
 C, d = model parameters, and
subscripts = time step denotation.

Generally, an increase in flow results in an increase in solid and dissolved loads. But a high value in suspended solids content does not have the same significance in rising discharge as in falling discharges.

In rising discharges, the proportion of runoff water which contains suspended material from soil erosion is greater than in falling discharges - periods where water comes more from underground flows.

The origin of water could also explain typical variations of water quality parameters found in many rivers. For example, J. Davis and H. Keller have demonstrated cyclic behaviors of relationships between concentrations and discharges (fig. 3 and 4) for both large and small basins. But in addition to the main factor which is likely to be water origin, the seasonal cycle could also be influenced by the temperature regime and the hydrobiological cycle. This is particularly true for parameters such as nitrate or silicate concentrations. Temperature has a definitive effect on chemical and biological reactions, and in waters where there is sizeable primary production,

Suspended solids (mg/l)

Rhine at Koblenz

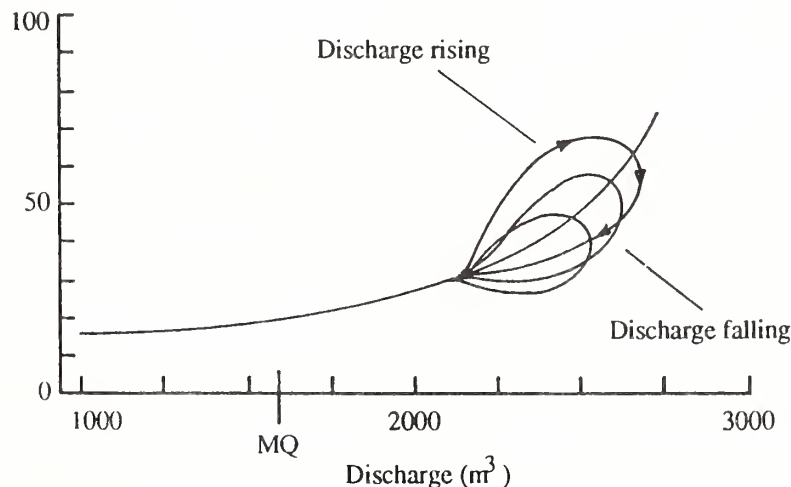


Figure 2.
Relation between
suspended solids content
and discharge.

nutrient compound concentrations react to the growth of aquatic plants and algae. Figure 5 shows, for example, an apparent relationship between nitrate concentrations and discharges. Figure 3 confirms this observation, and additional information such as the seasonal cycle. It was determined that for the same discharge, NO_3 values are higher in spring than in fall where part of the nutrients have been used by phytoplankton.

To summarize this first discussion:

- (1) there is a definite relationship between water quality parameters and discharge;
- (2) water quality is likely to be governed by point of origin;
- (3) water quality is also dependent on internal processes such as hydrobiological cycles, and processes related to quantitative aspects such as bed and bank erosion and sedimentation; and
- (4) for these reasons, peripheral considerations are needed to understand the significance of a set of data on water quality.

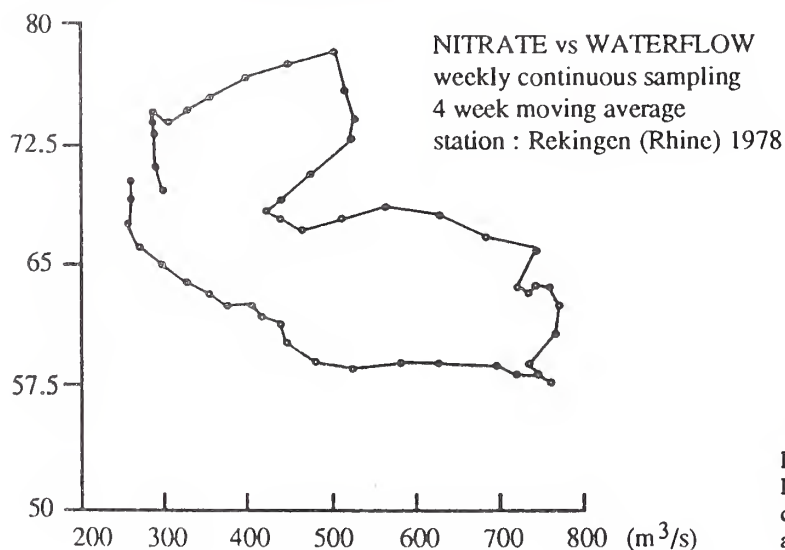


Figure 3.
Relationship between Nitrate and
discharge for the Rhine at Rekingen
after Davis and Keller (1983).

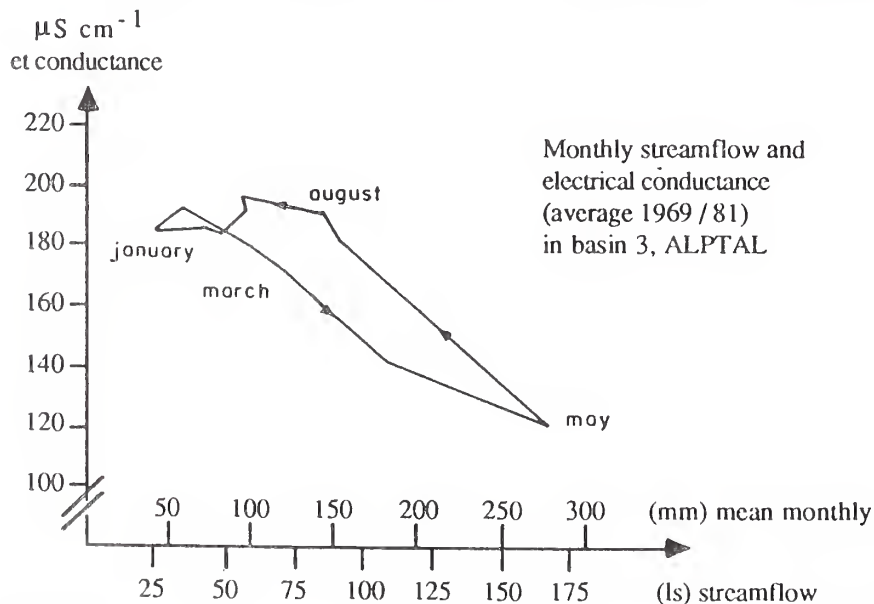


Figure 4.
Electrical conductance as function of flow; after Davis and Keller.

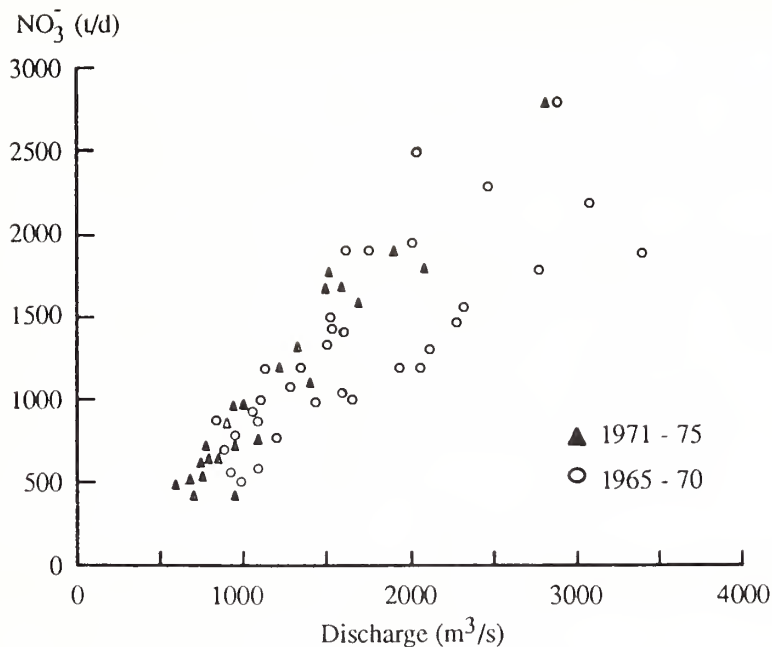


Figure 5.
Correlation between transport and discharge in the Rhine at Kaub after H. Hellmann.

RELATION BETWEEN WATER QUALITY AND QUANTITATIVE ASPECTS RELATED TO HYDRAULIC PROJECTS OR WATER MANAGEMENT

In natural waters, water quality parameters are somehow associated with quantitative aspects such as discharge and associated parameters like water velocity and depth. As we have seen, the change in water quality with discharge results partly from the origin of water and partly from internal processes such as erosion of bed and banks, sedimentation and chemical or biochemical reactions as well as physiological processes such as algae or aquatic plant growth.

Artificial control of discharge, for example through the operation of a reservoir, is likely to have different effects on water quality than natural variations. Generally, hydraulic projects alter certain physical parameters which have a substantial influence on water quality and, therefore, on the ecosystem. Despite the diversity of these projects, general laws can be established by studying the physical parameters changed, and the consequences of these changes on water quality.

The discussion below will be limited to the study of a few general parameters which provide a good picture of water quality and aquatic life, such as temperature and dissolved oxygen.

The impact of hydraulic projects or of their management upon quantitative parameters can be summarized by:

- (1) alteration of discharge,
- (2) alteration of water velocities,
- (3) alteration of water depth,
- (4) change in the residence time of water mass within a given river stretch, and
- (5) geomorphological changes.

The alteration of discharge acts locally, through the ability of the stream to dilute effluents. An increase in the rate of flow reduces concentrations by dilution. Generally the oxygen balance will

not be affected by oxygen exchanged with the atmosphere or the bed through absorption by sediment but will be affected by increases or decreases in flow rate. An increase of discharge in a more or less natural drainage basin increases the transport of suspended and dissolved substances; but if discharge increase has an artificial origin such as from regulated reservoirs, the transport of substances may not be increased either because sedimentation occurred in the reservoir or because water originally stored had a lower load. Fluctuation in discharge is likely to reintroduce suspended matter. The effect on water quality will involve not only suspended material, but many other parameters. Since suspended matter affects light penetration and associated eutrophication processes, it has a direct impact on aquatic life - even fish populations - and it is a major means of transport for many toxic components like heavy metals, radionuclides, and bacteria.

Water velocities play a major role in sedimentation mechanisms and resuspension of deposits. In general, a decline in velocity favors sedimentation of suspended mineral and organic substances including plankton, and therefore should reduce turbidity. It should be noted that gaseous exchanges at the surface are a function of the relative velocity between air and water. A decrease in water velocity reduces oxygen flux with the atmosphere. In practice, however, such exchanges are mainly governed by wind speed (which is likely to be higher than water velocity) so alteration of water velocity usually has a small or negligible effect on gas exchanges.

The reduction of water velocity of streams can favor formation of local stratification in deep reaches, thus internal exchanges within the water body are reduced. This may induce local growth of phytoplankton and sometimes anaerobic conditions in the vicinity of the bed. Fish populations are influenced by flow conditions. High-velocity currents are beneficial to some species while other species prefer somewhat stagnant waters. The change in sedimentation affects the benthic population and the potential of certain zones as spawning grounds.

The depth of a stream conditions the thermal inertia of a water body. Assuming that the turbulence generated by the flow is sufficient to make the stream vertically homogeneous, increased depth reduces daily temperature fluctuations caused by solar radiation or more generally by weather changes. At a seasonal level, the thermal behavior is practically independent of average depth. Average depth can alter the oxygen balance of a stream since the oxygen flow exchanged at the surface is distributed over a different volume. The same is true of oxygen losses from sediment oxygen demand and plant respiration. Increased depth will favor plankton growth to the detriment of benthic flora since less solar radiation reaches the bottom. Another aspect to be borne in mind relates to fluctuations in water level which are, in general, harmful for certain species of benthic invertebrates and can adversely affect spawning.

In practice, changes in residence time are a consequence of changes in the parameters discussed above. These physical parameters probably have the greatest influence on water quality, because time plays a fundamental role in the kinetics of nearly all chemical and biological processes. Most hydraulic projects increase the transit time of water in the zones of interest except, for example, when low flows are increased. Depending on the initial state of the stream (which may be cold, warm or at local temperatures, Gras et al. 1983) an increase in residence time can change thermal behavior. For example the temperature of incoming water moves to the natural local temperature, i.e. to the temperature of a stagnant water body of the same depth and subject to local meteorological conditions.

The dissolved oxygen balance can be substantially modified by residence time, especially in a relatively polluted environment. This balance results from a set of chemical and biological processes (including biological degradation of organic substances, benthic oxygen demand, gaseous exchanges at the surface, photosynthetic production of oxygen, the nitrogen cycle, etc.) whose kinetics are influenced to a varying extent by time. In practice, it is impossible to generalize whether the increase in residence time produces a decrease or an increase in oxygen content. Increases in some zones and decreases in others may occur along the same stream. The increase

in residence time can favor plankton growth. In extreme conditions, plant growth in primary production can change from a system in which plants are attached to the bottom and banks, to a purely planktonic system.

EXAMPLES OF WATER QUALITY EFFECTS OF HYDRAULIC PROJECTS

River Channelization

Channelization of rivers generally involves modifying banks, deepening certain zones, and often creating reaches where water velocities are decreased and residence time lengthened. It is thus to be expected that this type of development will have a substantial effect on the local environment.

Change in water depth implies a change in thermal inertia. Nevertheless, the effect on thermal behavior often remains limited to a reduction in the amplitudes of diurnal cycles and short-term fluctuations. This is valid especially for lowland rivers which are already in equilibrium with local meteorological conditions (fig. 6).

Since the rate of flow is not affected by such a development, the physical and chemical parameters will be indirectly influenced by the action of the change in water velocity and depth, for instance sedimentation and planktonic growth. In general such a project promotes a changeover from benthic flora to a phytoplanktonic system (fig. 7). This changeover will be enhanced by pollution associated with domestic effluents as well as agricultural practices. Fish resources will certainly be highly modified, but with greater impact on the structure of population than on biomass production. Aesthetic effects comes from the change towards phytoplanktonic life.

The final effect on channelization results from the combination of various processes whose effects may be contradictory. Concerning eutrophication, the role of suspended matter is important. Reducing velocity is likely to increase sedimentation and thus increase light penetration by reducing suspended material, however increase in depth tends to reduce light in the water column. Figure 8 shows another way of studying combined effects on phytoplankton growth of suspended matter, depth, longitudinal evolution in the river and discharge.

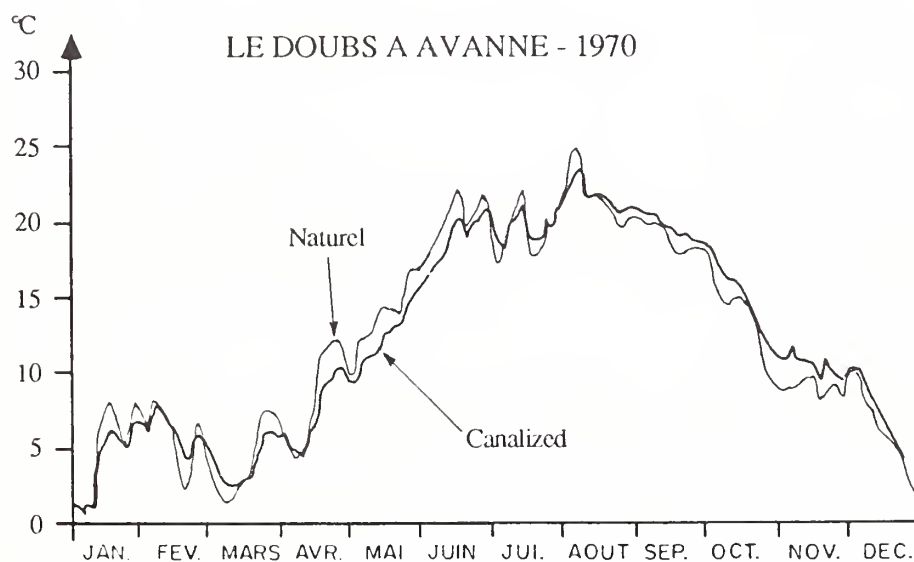


Figure 6.
Change in Doubs River thermal behavior due to channelization (actual and after channelization, with the same weather conditions) based on a simulation model.

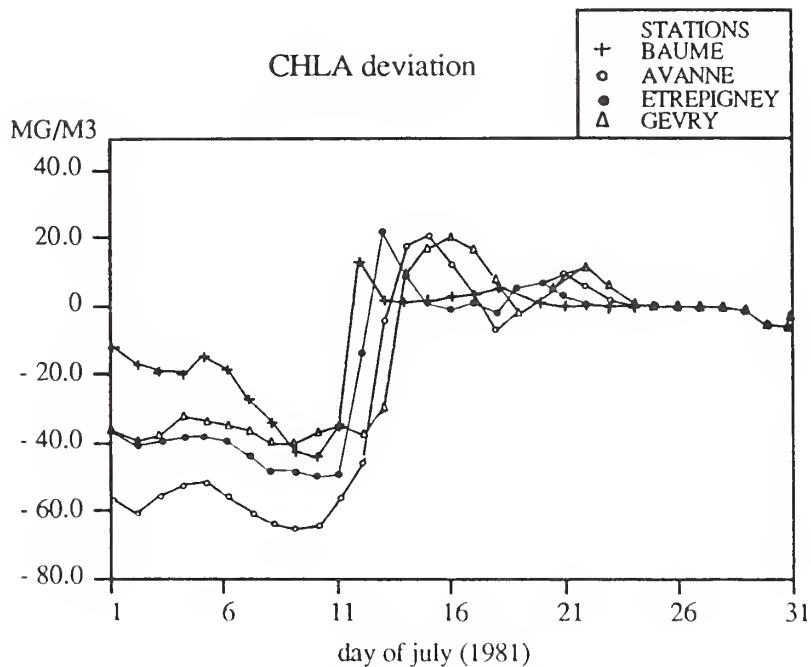


Figure 7.
 Effect of channelization on phytoplankton growth. Difference between chlorophyll a concentration after channelization and before for the Doubs river for various stations (for a typical month).

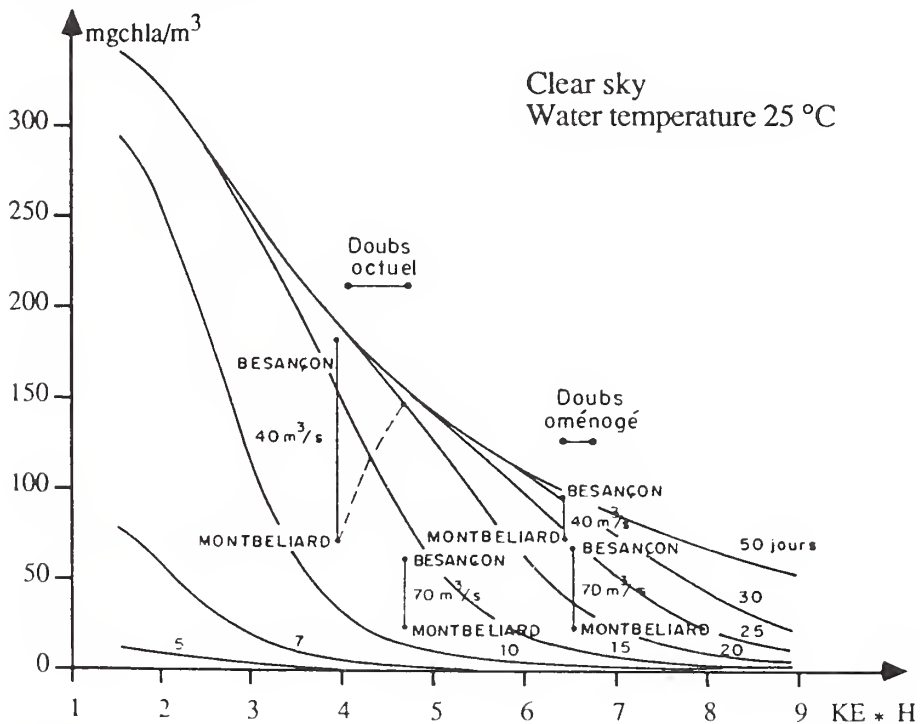


Figure 8.
 Potential biomass of phytoplankton as a function of water transparency (KE-light extinction coefficient in water [m⁻¹] and water depth H [m] for various residence times. These model results are given for good weather conditions and a water temperature of 25°C. Evolution of phytoplankton concentration in the Doubs river between Montbéliard and Besançon are given for two discharges for the present stage (Doubs actuel) and projected stage (Doubs aménagé).

Creation of Reservoirs

The creation of a reservoir in a drainage basin, involving modification of the rate of flow and the water quality has a direct effect on the submerged part of the drainage basin and an indirect effect downstream from the dam. It is of interest to consider, in broad terms, the change induced by water impoundment. This change will be of most importance when the characteristics of the reservoir approach those of a lake, i.e. when water residence time is long. The biggest differences between a lake and a river are the river's capacity to renew water and the possibility of lake stratification. In these terms, a reservoir is an intermediate environment between a lake and a river. The reservoir will become similar to one or the other of these two environments, depending on depth and residence time. The influence which the creation of a reservoir has on the water quality and aquatic life of a river will now be discussed according to length of the residence time.

Reservoirs with Short Residence Times

When residence time in a reservoir is short (a few days), there is almost no stratification, except in special cases such as deep reservoirs with a cold inflow and with water withdrawal from near the bottom. The influence on temperature of reservoirs with short residence times consists of a reduction in short-term fluctuations (diurnal cycles, changes in meteorological conditions), but the alteration of water quality will mainly concern the deposition of suspended matter. A changeover from benthic primary growth to planktonic production may be observed and components of the oxygen balance can be slightly modified. Surface aeration will be reduced and benthic oxygen demand will depend on the nature of sediment deposits (in general, an increase in the value of this term can be expected). A rise in residence time, even of a few days, may have a marked effect on the biodegradation processes involving an increase in the oxidation of organic matter including detritic plankton, although the latter will increase the quantity of organic matter to be degraded downstream.

Reservoirs with Long Residence Time

When residence time increases, summer stratification is more easily developed. The water quality and the characteristics of the ecosystem as a whole approach those typical of a lake. The surface layers become progressively isolated from the remainder of the water body as stratification develops. Planktonic life takes over from benthic primary production. The sedimentation terms increase and the reservoir traps mineral and organic matter. Exchanges at the bottom take on greater importance and increased oxygen demand. Release of nutrients or heavy metals may occur when physico-chemical conditions become anaerobic. There is thus a thorough change in the water quality as well as in aquatic life as a whole, ranging from the initial links of the trophic chain to fish. Population structure will differ markedly from that of a stream although this does not necessarily imply a reduction of biomass; in fact the reverse may occur (Brossard and Gallene 1982).

Downstream as well, a marked effect on the water quality and aquatic life, at least in the vicinity of the dam, may be expected. In practice, the water quality in the reservoir - like that of the water withdrawn, which consequently feeds the downstream section of the stream - depends on the management of the system:

- (a) either through the design of the facility itself, including the level at which water is withdrawn and shape of the intake, which have an effect on the layers of water withdrawn, or,
- (b) the quantitative management of water, including the period during which the reservoir is filled and the downstream rate of flow and fluctuation.

It should be noted that even reservoirs with long residence times are likely to drastically modify water quality. They offer tremendous opportunities to control downstream water quality, in particular if they are equipped with multilevel outlet structures.

WATER QUALITY, USES, OBJECTIVES, AND CRITERIA

To judge the quality of something pre-supposes that criteria have been selected for that purpose. The main difficulty comes from the fact that criteria vary from one use to another and are often in conflict. Water which is suitable for a given use may not be acceptable for other uses. Even for the same use different criteria may be in conflict. For instance, in the case of fishing, water quality should satisfy characteristics for fish production both in terms of biomass and structure of fish population. In some countries cold streams are preferred for fishing since this environment favors salmon type of fish, but in contrast biomass production is low under such conditions. Swimming requires a low bacteriological level and high water temperature. Whereas abundant plankton life is likely to give a color and turbidity which swimmers find unpleasant, photosynthesis associated with phytoplankton improves the bacteriological quality of the water through oxygen production. This illustrates the fact that criteria may be conflicting for the same use. Conflicts between uses are so common that they should almost be considered as the rule.

So managers of water quality are supposed to have users to protect and define objectives. For each use it is necessary to establish criteria for measuring water quality. Criteria vary from use to use and could be described by various parameters or combinations of parameters. For instance, navigation requires mainly consideration of physical parameters such as water depth and sometimes water velocity, while criteria related to drinking water are mostly physicochemical parameters or bacteriological parameters. It is clear that criteria or parameters to measure water quality of a water body are so numerous that it will not be practicable to consider all of them and we should restrict ourself to consider only those associated with the uses of concern for that water body.

Criteria can define parameters that are a means of measuring water quality, but to put a judgement on quality we need standards. Again it is important to recall that standards should also be appropriate to the water body; considering specific uses and objectives. In that respect, it would be unwise for a country to adopt foreign legislation without considering its own objectives and context. For example, a fight against lake eutrophication may be a proper objective for some countries where food is abundant, but eutrophication processes may sometimes be considered beneficial within certain limits due to a compromise between different uses or objectives: fish production, fish species, aesthetic questions, public health, etc. Ponds of fish farms are often extremely eutrophic in order to increase production.

According to paragraph 3, section 10 of the U.S. Federal Water Pollution Control Act:

"Standards of quality established pursuant to this subsection shall be such as to protect the public health or welfare, enhance the quality of water and serve the purposes of this Act. In establishing such standards the Secretary, the Hearing Board, or the appropriate state authority shall take into consideration their use and value for public water supplies, propagation of fish and wildlife, recreational purposes, and agricultural, industrial, and other legitimate uses".

This does not imply that water quality should be suitable for all these uses simultaneously, but specific standards are to be defined according to each type of use. The European Community also has set water quality recommendations for specific uses such as drinking water and aquatic life.

Another point is related to the type of parameters used to describe water quality. Chemical parameters are commonly considered necessary to measure water quality. It is not so obvious for

physical parameters, although no one will disagree on parameters such as temperature and conductivity, but what about depth and velocity for a river? I understand that these parameters are only to be considered for specific water bodies and specific uses, but water depth and water velocity are, for some rivers, more decisive factors than temperature or conductivity since they control fish habitat. Fish habitat is related to fish production, fish population structure, and benthic fauna or flora. Parameters describing water quality should include physical, chemical, and biological factors. Many water uses are greatly affected by biological life. These include not only public health which is mostly concerned with bacteriological life, but also recreational activities such as fishing and swimming which are very sensitive to the eutrophication state of the waterbody. Other water uses such as water treatment plants for drinking water are also affected by biological life. Their operation may be altered by the growth of certain algal species (such as blue algae) which impart an unpleasant taste to drinking water. It is easier to estimate phytoplankton concentration than to consider all of the elements responsible for, or to control phytoplankton growth. Why consider dissolved solids load or sediment load as water quality parameters and not concentrations of anabaena, anacystis, microcystis or chlorella algal species which produce toxins and are therefore very important?

There are two ways to set standards. The first is to consider how and when a given use could be properly satisfied. For example, what water quality standards are suitable for human consumption or livestock supply? This type of standard is established to protect the user by insuring a minimum level of quality; for example, swimming water should be warm enough, clean enough, have little turbidity as possible (which means not too much suspended material or algae) and should be bacteriologically acceptable. Table 3 is intended to present the list of qualities on which requirements may be established to satisfy a given use.

Use of water is not free. Often, if not always, water use is likely to alter some of its qualities. For example, the use of a river as a pollution vector, say for domestic sewage or industrial waste waters, will alter its oxygen content, and its chemical composition, it may increase the number of pathogenic organisms, and favor eutrophication processes. Table 4 lists for each use, water quality parameters which are likely to be modified by this use.

The second aspect standards are controls to avoid a given use impairing other uses. This second way of setting standards intends to solve conflict between uses and is based on various objectives which may of course vary from one country to another, and also from one water body to another. These objectives result from a compromise and are subject to arbitrary decisions, therefore priorities should be defined between uses. The following simplified approach intends to show that there are basic considerations which should remain in any situation, and that the degree of liberty in setting standards lies not on parameters to be considered, but how high to set limits.

From tables 3 and 4 it is easy to see the interaction between uses. Table 4 shows the parameters affected by a given use and table 3 the parameters on which requirements are necessary for various uses. Table 5 gives the direct result of crossing table 3 and table 4. Of course a single parameter is not always drastically affected by a given use, and the requirements are not always stringent. Table 6 considers only the strongest interactions.

Who is going to reject the following priority list:

- (1) survive,
- (2) live,
- (3) live decently,
- (4) live well?

In other words, compare a very poor country to a very rich one. Each level of priority identifies different uses that must be satisfied. It appears (table 7 and 8) that in all cases a country has to

Table 3.
Water quality parameters on which certain requirements
are needed to properly satisfy a given use of water.

THIS USE

needs

THESE QUALITIES

Criteria Uses	Physicochemical				Biology			Morphodynamical parameters		
	T°C	O ₂	N P Si	Toxic	Bacteriology	BOD	Eutrophication Level	V	h	Q
Navigation									X	
Fishing	X	X	X	X			X	X	X	
Swimming	X	X		X	X		X			
Canoe, kayak					X			X	X	X
Drinking water	X		X	X	X					
Pollution vector										X
Cooling	X									X
Chemical processes	X		X	X		X				
Aesthetics						X	X	X	X	X
Irrigation			X							
Change of drainage conditions										

fight first against water pollution (domestic pollution, then industrial pollution and then agricultural pollution). The environment is not a toy for the rich but a concern for everyone. Putting this idea in other terms - there are virtually no situations where the concept of a water resource does not include water quality as well as water quantity.

Although based upon general objectives, standards should maintain a minimum value and cannot be totally adapted case by case or they will be unable to play their role of safeguard. Nevertheless, local objectives may need to be established in order to maintain or reclaim a certain level in water quality. It is technically and politically easier to maintain a good level in water quality than to restore a satisfactory level when pollution has reached too high a level.

Before setting objectives, water quality must be monitored. This may appear to be a waste of time and money since it does not correspond to abatement action. In fact, water quality monitoring constitutes an indispensable step in pollution control for two reasons. The first is to get a clear perspective of the problem in terms of type of pollution and its magnitude, to localize critical areas, etc. The second reason is that monitoring permits one to determine the consequences of actions which are undertaken.

Table 4.
Water quality parameters which may be affected by given uses of water.

THIS USE needs THESE QUALITIES

Water quality parameters Uses	Physicochemical				Biology			Morphodynamical parameters		
	T°C	O ₂	N P Si	Toxic	Bacteriology	BOD	Eutrophication Level	V	h	Q
Navigation	X	X		X		X	X	X	X	
Fishing										
Swimming					X					
Canoe, kayak										
Drinking water										
Pollution vector		X	X	X	X	X	X			
Cooling	X	X								X
Chemical processes	X	X	X	X		X	X			X
Aesthetics										
Irrigation			X				X			X
Change of drainage conditions		X	X	X	X	X	X			X

The second step is to fix objectives in terms of the level of water quality to be reached. For a river, this should be established reach by reach. This step should be sufficiently realistic so that the program is politically and financially feasible.

The last step consists of defining priority actions, since it is not possible to eliminate all pollution sources at once. Mathematical models will be of help in examining various strategies.

For example in figure 9 the fight against eutrophication on the Moselle river between the Meurthe river mouth and the city of Thionville is examined. This stretch of river receives many large industrial and urban discharges and the level of eutrophication is very high. A model has been built to study the consequences of various actions. Figure 9 shows the results of the study. Today it appears that phosphorous content of the Moselle river upstream is not limiting plant growth, therefore, a reduction of phosphorus discharge in this highly polluted stretch will not immediately affect eutrophication levels. Money spent to reduce phosphorus content will appear to the public as money wasted. It is therefore more useful to first reduce phosphorus content in the upper river, although it is not the most polluted area.

The purpose of this meeting concerns water quality in relation to agricultural practices, this problem has two facets. The first concerns water quality for agricultural uses. The second deals

Table 5.
Interactions between various uses of water in relation with water quality (schematic).

USES→	Naviga- tion	Fish- ing	Swim- ming	Canoe, kayak	Drinking water	Pollution vector	Cool- ing	Chemical process	Aesthetics
Navigation		X	X		X	X	X	X	
Fishing	X	X				X	X	X	
Swimming			X	X	X				
Canoe, kayak									
Drinking water									
Pollution vector		X	X		X	X		X	X
Cooling		X	X	X	X	X	X	X	
Chemical processes		X	X	X	X	X	X	X	X
Aesthetics	X					X		X	
Irrigation		X		X		X	X		X
Change of drainage condition		X	X	X	X	X	X	X	X

Table 6.
Interactions between various uses of water in relation with water quality.

OF → ON	Naviga- tion	Fish- ing	Swim- ming	Canoe, kayak	Drinking water	Pollution vector	Cool- ing	Chemical process	Aesthetics
Navigation		○	○	●		○			●
Fishing		○				●	○	●	
Swimming			○						
Canoe, kayak									
Drinking water									
Pollution vector		●	●		○	●		○	●
Cooling		○	○		○	○	●	○	
Chemical processes		●	○		○	●	○	○	○
Aesthetics	●					●		○	
Irrigation						○			
Change of drainage condition		○	○			○			○

○ Significant impact ● Large impact

Table 7.
Simplified priority criteria between water uses.

① First survive!	→	• drinking water • public health • irrigation	(bacteriology)
② To live	→	• drinking water quality • commercial fishing	(reservoirs, river flow) (improving biomass)
③ To live decently	→	• economical resources	- industrial uses - navigation
④ To live well	→	• leisures - aesthetics • nature preservation.	- swimming, fishing, sailing, canoe ...

Table 8.
Sources of pollution that must be controlled to meet criteria of table 7.

PRIORITY		→	CARE ABOUT	
① First survive	→	○ Pollution ○ Industrial waste waters	(domestic)	
② To live	→	⊗ Pollution ⊗ Industrial waste waters ○ Navigation ○ Drainage conditions ○ Fishing	(domestic)	
③ To live decently	→	⊗ Pollution ⊗ Industrial uses ○ Drainage conditions	(domestic)	
④ To live well	→	⊗ Pollution ⊗ Industrial uses ⊗ Navigation ○ Drainage conditions ○ Fishing, swimming.	(domestic)	

with the impact of agricultural practices on water quality, and how to protect other uses, or how to protect agriculture from itself. The latter is most important for irrigation water supplies in arid zones.

Water supplies for agricultural uses are commonly divided into three groups by need:

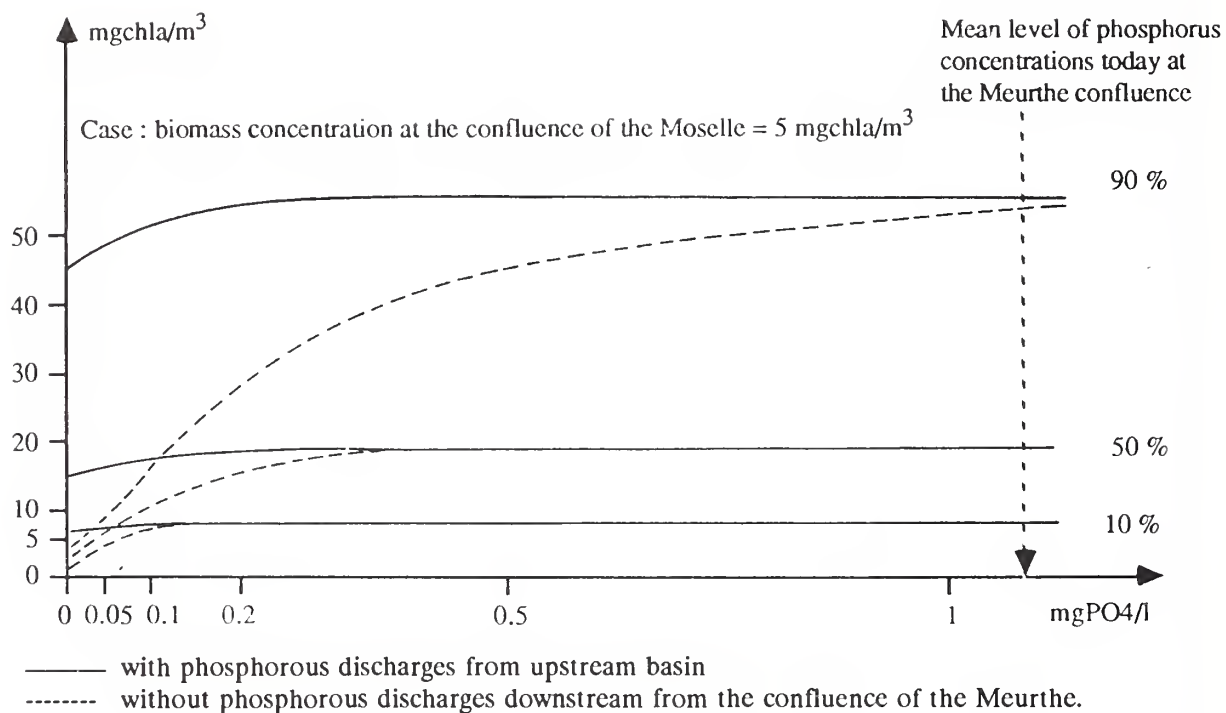


Figure 9.
Statistics of phytoplankton biomass at Koenigsmacker as a function of total phosphorus concentration at the confluence of the Meurthe and the Moselle rivers.

- (1) water for farmstead uses such as drinking water, household water, raw agricultural commodities and milk sanitation,
- (2) water for livestock, and
- (3) water for irrigation.

Requirements are, of course, very different from one use to another setting standards or guidelines for farmstead water supplies is certainly easier since water is partially used for drinking and milk sanitation. Finding a proper source or an appropriate water treatment is a problem to be solved locally. Standards here are directed to insure water is suitable for the use in question.

Livestock water supplies do not require water quality standards as high as those for human consumption. In general, the risk of toxicity is less from water than from feed sources. This is why there are no strict standards set for livestock water. In some cases, water quality standards are set to conform with acceptable residual levels in marketable animal tissues or products (for example concentrations of toxics in milk) rather than in relation to toxic affect upon the animals themselves.

Standards or guidelines set for irrigation water intend to serve two different goals. The first goal is to insure water quality for irrigation which is suitable for growth of specific plants. Tolerance to salt varies greatly among plants, the effect of salt being first a reduction of yield and eventually complete plant growth inhibition. The other goal pursued by irrigation water quality standards or guidelines is to insure proper irrigation management. For instance, recommendations on suspended solids may be wise in order to avoid crust formations on the soil surfaces which reduces seedling emergence, infiltration, irrigation efficiency, and hinders leaching of saline soils.

Water used for agricultural purposes is likely to alter water quality of both groundwater and surface water systems. Three main factors are responsible for these changes:

- (1) Irrigation or even non irrigated farming can modify the natural water cycle changing run off, evapotranspiration, infiltration, and drainage conditions. This is likely to modify erosion processes and dissolved solid loads of ground and surface waters. A main concern, especially in arid zones, is the question of soil salinization.
- (2) Extensive use of fertilizers is likely to increase the nutrient loads of surface waters and lead to eutrophication of rivers and lakes.
- (3) Pesticides (such as insecticides, fungicides, rodenticides and herbicides) are widely used and are likely to be exported by the water systems; some are subject to rapid biodegradation but, some degrade extremely slowly.

A common point of all these alterations of water quality lies in the fact that all are nonpoint pollution sources. There are political and socio-economical constraints which sometimes render these more difficult to control than a point source; it is also technically easier to control point source pollution. When dealing with nonpoint pollution the relationship between the source and the receiving water is complex and not always fully understood.

Mechanisms which are involved in this relationship cover a range of physical, chemical and biological processes. First, however, it is important to understand the water cycle from runoff (overland and channel flows) to evapotranspiration, infiltration and storages. Then the physical processes related to soil erosion, which also are significant in water quality alteration, must be understood. This includes soil detachment by raindrops, overland flows, loose soil storage, deposition, and resuspension of deposits in channels. Chemical and biological processes that intervene at various levels, adsorption and desorption of pollutants on suspended matter, and fate of fertilizers in ground and surface water as affected by chemical or biological processes.

Modeling seems a necessity to properly explain the complexity of these phenomena. But today knowledge is only sufficient to build descriptive models which provide answers on how systems react or more exactly, give tendencies of reaction to a given modification. Models dealing with sediments are mostly designed for computing or estimating yields on a time basis too long for studying water quality.

Recent dynamic models and stochastic models may provide rather detailed information such as particle-size composition for specific hydrologic events. They require a comprehensive set of data for the drainage basin and are applicable to small watersheds. A few models have been made to model nitrogen transport and transformations in soils: these models are applicable only for small-scale basins.

CONCLUSION

For a long time, water management has been mostly a question of quantity; for many reasons, water quality did not constitute a primary objective. Benefits drawn from a good water quality level in rivers and lakes as well as groundwaters were not very obvious for most uses, especially at a time when water supplies of acceptable quality were readily available. Interest in water quality only arose with the increase in water degradation and the decrease in available water supplies of acceptable quality. It is difficult to justify spending money on a project without immediate and obvious benefits.

To consider water quality properly, it is necessary to study not only parameters directly connected to the use or uses of concern, but also to analyze the surrounding conditions. Discharge is a decisive factor influencing quality parameters in a river, but groundwater may be affected by recent weather conditions or the type of crops, and on a more general basis by land use. What is true for natural or nearly natural rivers is also true for artificially controlled systems. Apparently harmless projects designed for quantitative water-resources management may alter if not impair water

quality. Operation of hydraulic projects is likely to induce changes in water quality, thus water quality objectives may be achieved or at least taken into account by operating procedures. Conversely, water quality concerns may have an impact on quantitative aspects by reason that quality objectives may impose quantitative constraints.

Diffuse pollution comes essentially from agricultural practices and small urban or uncontrolled industrial discharges. Controlling this type of pollution is technically more difficult than controlling point-source pollution because it necessitates not only technical measures, but political ones as well. For example, rational use of fertilizers and pesticides is not necessarily obvious and requires some technical skill. The receptiveness of farmers to scientific arguments varies with country and region. Also a compromise should be found between standing crop benefits and pollution control. Many different approaches can be found to achieve a specific policy: control the cost of fertilizers and pesticides, impose taxes on products or on use of water, and distribute information about adequate agricultural practices in order to reduce pollution.

Interaction between water quantity and quality is inevitable, because vital water uses require good quality. It is easier for technical, financial and political reasons to maintain an acceptable level of water quality than to restore it after degradation. It appears that water quality should be a constant concern for all people dealing with water resources or working on any project which may interact with the water system.

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DISCUSSION OF KEYNOTE ADDRESS - PUTTING WATER QUALITY INTO PERSPECTIVE - QUALITY VERSUS QUANTITY BY DR. RAYMOND A. GRAS

Bruce Bishop¹, Presiding
Darwin Sorensen², Recorder

TITLE

Putting Water Quality Into Perspective - Quality versus Quantity by Dr. Raymond A. Gras

SUMMARY

One question was asked (by an unidentified audience member) about how the French society deals with conflicts between pollution control (e.g., waste load allocation) and multiple uses of water in different segments of society.

Dr. Gras (President, International Water Quality Commission, Electricite de France, Chatou, France) thought that, because of the lack of clarification of what multiple use includes, resolving conflicts between water quality and water uses is difficult. A lot of agencies deal with water quality both in France and in the U.S. Often the responsibilities of the agencies are primarily financial and not scientific. Dr. Gras did not feel that there are, necessarily, conflicts among agencies dealing with water but the responsibilities are distributed within and among the agencies. In his opinion, the multiple use of water is a matter which is difficult and is a problem that has not been properly resolved. The problem is not unique to France, but occurs nearly everywhere.

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CHEMICALS IN WATER: GETTING A HANDLE ON HEALTH RISKS

Chris F. Wilkinson¹

ABSTRACT

A large segment of the U.S. public believes that residues of synthetic chemicals in food and water are responsible for significant adverse effects on human health. However, there is no evidence to support this view for either acute toxicity or for chronic effects such as cancer. While the presence of any chemical in water should always be carefully evaluated, the levels of chemicals currently present in U.S. drinking water are below those likely to constitute any significant threat to human health.

INTRODUCTION

No one can dispute the fact that an adequate supply of potable water is an absolute prerequisite for healthy living. Conversely, "bad water" has long been associated with illness and death, and water-borne diseases such as cholera and typhoid continue to take a massive toll of life in many of the less developed countries in the world (van Damme 1985). Such diseases were rampant in Europe and the U.S. only a little more than a century ago as a result of the contamination of drinking water with raw human sewage, and it is of interest to note that there are still some 40 outbreaks per year of diseases such as salmonellosis, shigellosis, giardiasis, etc. (Harter et al. 1985). As a consequence, most of the early U.S. legislation to control water quality was focused on preventing the spread of disease.

But raw sewage has not been the only form of human waste that has found its way into our surface waters. It seems that rivers, lakes and ponds have always provided convenient receptacles for just about any kind of waste produced by society -- out of sight, out of mind. Since the nature of human waste is largely a reflection of contemporary technology, it is perhaps not surprising that, for a number of years, chemical pollution increased in a way that followed the rapid growth of the chemical industry. There is no question that as a result of ignorance, thoughtlessness, negligence and poor judgement, some serious mistakes were made. Thousands of tons of chemical products, byproducts and wastes were purposely or inadvertently released into the environment. Much of this ultimately found its way to water. We have all seen the results of these mistakes in the grossly polluted surface waters of many of our urban ecological disaster zones. Clearly, surface waters have always been highly vulnerable to all types of pollution and from the 1920s through the 1960s there was increasing U.S. legislation to address health concerns associated with the presence of bacteria, inorganic chemicals and radioactivity in drinking water.

The potential health problems associated with organic chemicals in drinking water received little or no attention until 1974 when the 93rd U.S. Congress passed the Safe Drinking Water Act (SDWA). In part, this Act required the EPA:

1. to work with the National Academy of Sciences (NAS) to develop a series of recommended maximum contaminant levels (RMCLs) [subsequently changed to maximum contaminant level goal (MCLG) in the 1986 Amendments to the SDWA] that would serve as health-based goals for all types of drinking water contaminants,

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2. to develop maximum contaminant levels (MCLs) that would be regulatory standards as close as technically feasible to the RMCLs and
3. to develop a series of health advisories (HAs) for emergency situations.

During the period when the SDWA was being formulated, the environmental movement in the U.S. was in full swing -- the spotlight of national concern was focused on chemicals, particularly pesticides and industrial waste. Indeed, it was, in part, sorry sights such as heavily polluted waterways and resulting fish kills, etc. that first generated public concern and created the initial impetus for the environmental movement in the early 1960s. During the late 1960s and early 1970s, however, the main focus of attention shifted away from the highly visible environmental impacts of pollution to the invisible, largely unknown effects of chemicals on human health. Passage of the health-based SDWA in 1974 was right in line with this tilt in public concern and it was not surprising that the first interim primary drinking water standards for organic chemicals were for six pesticide chemicals.

By 1986, the EPA had developed standards for only 25 pollutants in drinking water but had proposed RMCLs and MCLs for about 50 other inorganic/organic materials. Regulatory activity was markedly increased by the 1986 Amendments of the SDWA that required the EPA to speed up the promulgation of standards for these and other contaminants to a rate of about 25 every three years.

PUBLIC CONCERN

Unfortunately, passage of the SDWA and the volumes of other federal and state legislation aimed at protecting human health and/or the environment, seem to have done little to calm the public's fears. Indeed, if anything, the situation is getting worse. Today, a large segment of the general public is convinced that traces of synthetic chemicals, particularly pesticides, in our air, food and water are linked directly with cancer, birth defects and a host of other human ills.

It seems as though we like to worry. Despite the fact that we are living longer and that our health and the general quality of our lives is better than ever before it appears that, as a society, we have become obsessed with the risks in our lives. Certainly the fear and worry that exist out there are very real. People are afraid and confused and many are, indeed, worrying themselves ill, over risks very much smaller than those we face driving to work each day. As a society we seem to have lost our ability, if we ever had it, to distinguish between truly serious risks and those of a quite trivial nature. We are also irrational in selecting the things we worry about. We smoke billions of cigarettes a year and yet we are quite paranoid about traces of pesticides in our food or water or artificial sweeteners or food additives calculated to cause at very worst a 1 in 1 million risk of cancer.

THE GROUNDWATER ISSUE

The discovery, in the late 1970s, that groundwater in some parts of the country was contaminated by pesticides further heightened public concerns over chemicals, and subsequent well-publicized reports of the presence of solvents and other chemicals in groundwater has reinforced the impression that we are facing an imminent human health crisis. Groundwater protection has become a popular bandwagon issue.

There is no question that the widespread contamination of groundwater constitutes a legitimate national concern. Some 85% of the total water resources in the U.S. is in the form of groundwater aquifers, and groundwater provides drinking water for about 50% of the U.S. population; in rural

areas some 95% of the people get their drinking water from ground water. While we have always accepted the vulnerability of surface water to contamination from human activities, we have generally considered groundwater to be safe and pure. Understandably then, the discovery that this is not always the case has come as something of a shock.

The resulting increase in regulatory and legislative action at both the federal and state levels was entirely predictable. The EPA has released its "Agricultural Chemicals in Ground Water: Proposed Pesticide Strategy" (EPA 1987) and the National Ground Water Research Act" of 1987 (H.R. 791), already passed by the House, proposes a comprehensive interagency effort to protect groundwater resources. In addition, state level groundwater legislation has already been passed in CA, WI, FL, NE, IA and MS; the issue of ground water protection has become highly politicized.

HOW BAD IS IT?

Before we throw up our hands resignedly in utter dismay, let's step back, take a good hard look at the situation and try to put things into better perspective. To what extent are our groundwater resources contaminated with synthetic chemicals?

Based on the nature and frequency of reports transmitted via the media, one might be led to believe that a large part of our groundwater is in real trouble. We have all heard about trichloroethylene in the wells of Silicon Valley, CA, and Woburn, MA, dichlorobromopropane in CA, ethylene dibromide in FL and aldicarb in Long Island, NY. We've heard about the problems of leachates from Love Canal and the Stringfellow acid pits, and we've all been exposed to local horror stories of leaking septic and gasoline tanks, ill-sited garbage dumps and illegal dumping. Such situations obviously represent a serious and very real problem for those who are directly affected. In total, however, these incidents involve only a relatively small fraction of our total groundwater resources, perhaps only 1 percent and certainly no more than 5 percent. The EPA has recently initiated the National Survey of Pesticides in Well Water in an attempt to define more clearly the scope of the potential problem that exists with agricultural chemicals; the results should be available in 1990.

As we shall see, even in the "hot-spot" areas where contamination has been identified, there is, as yet, little or no evidence to suggest that levels of chemicals having any significant adverse effects on human health have been reached.

ASSESSING HEALTH RISKS

Risk is a measure of the probability that an adverse effect will occur. In the case of a health risk from a chemical, it is a function of the intrinsic capacity of the chemical to cause some adverse effect (e.g., neurotoxicity or cancer) and the intensity and duration of exposure. The degree of exposure depends on the conditions under which exposure occurs. Clearly, with a pesticide, for example, the risks to an applicator are considerably greater than those to a member of the general public exposed to traces of the material in food and/or water.

Exposure

Unfortunately, for many, the very fact that a pesticide or other chemical is in water at all, at any concentration, is a cause for immediate concern. In most cases the chemicals in our groundwater are present in extraordinarily low concentrations that are usually measured in parts per billion (ppb). Despite the fact that concentration units such as ppm and ppb are used routinely by the media, there are very few people in the media or the public that have the faintest idea how big, or

rather how small, the units really are. Comparable proportions are shown in other more familiar units in Table 1.

A few years ago, we had great difficulty in measuring 1 ppm of anything. Now we routinely measure ppm and ppb and occasionally we can measure ppt (parts per trillion) and ppq (parts per quadrillion), one thousandth and one millionth of a ppb, respectively. We are fast approaching the time when we can measure just a few molecules. Our current analytical chemical capabilities are truly amazing, and the fact that they allow us to measure the smallest traces of almost anything we choose to look for, has tended to heighten public fears about the risks associated with traces of chemicals in our food and water. It tends to give the impression that we are wallowing in a sea of potentially dangerous chemicals. What we must remember is that we no longer live in a pristine environment. If we choose to use chemicals, particularly those like pesticides that are released into the environment by design, we will always be able to find traces of these in water, or elsewhere, if we have sufficiently sensitive analytical capabilities. Also, in conducting surveys we often tend to maximize our chances of finding chemicals such as pesticides by looking for them in shallow wells or water tables directly under the fields or orchards to which they were applied. In considering the possible health implications of such chemicals it might be more appropriate to conduct the analyses at the well head or at the tap to obtain a more accurate picture of the actual concentrations to which people are exposed.

The major problem, of course, continues to hinge not on detecting and measuring the traces of chemicals contaminating our ground water -- that's easy -- but on determining what, if any, biological significance they might have in terms of adverse effects on human health. Regulatory action cannot be justified simply on the basis of finding a given chemical per se, but only after carefully evaluating whether that chemical represents a potential health threat.

EPA Drinking Water Standards

The health effects of more than a hundred chemicals that may occur in water have now been evaluated and, working with the NAS, the EPA has developed MCLGs and MCLs for a number of volatile solvents, industrial chemicals and pesticides. Also, as required by the SDWA the EPA's Office of Drinking Water (ODW) has established a non-regulatory Health Advisory Program that provides information on the health effects of a number of chemicals that may occur in water. At the present time Health Advisories (HAs) for about 65 pesticides as well as a number of solvents have been prepared. They provide advisories on levels of chemicals at which adverse effects would not be expected following exposure for various periods of time -- one day, ten days, "longer" term, and lifetime. HAs are not legally enforceable standards. They are simply intended to provide guidance to federal, state or local authorities making decisions on the protection of public health.

Unfortunately, the EPA's MCLGs, MCLs and HAs are often interpreted incorrectly as toxicity thresholds, a fact that tends to exaggerate public fear for the actual health risks involved. Let's examine how these health-based standards are generated and what they mean.

TOXICOLOGY RISK ASSESSMENT

The major types of adverse effects of concern are usually described as either acute or chronic. Acute effects are those that occur within a relatively short time after exposure while chronic effects may occur months or even years after exposure. As far as the EPA is concerned, toxicology risk assessment is conducted in different ways depending on whether the chemical under consideration is or is not judged to be a carcinogen.

Table 1.
Comparable units of one part in a million and
one part in a billion.

<u>Unit</u>	<u>Concentrations</u>	
	<u>ppm</u>	<u>ppb</u>
Length	1" in 16 miles	1" in 16,000 miles
Time	1 min. in 2 yrs	1 sec. in 32 yrs.
Money	1 cent in \$10,000	1 cent in \$10,000,000
Population	1 person in a population a little less than that of Utah	1 person in China

Noncarcinogenic Chemicals

Assessing the potential noncarcinogenic effects of a chemical has never been much of a problem. This is because, for acute toxic effects, it is generally accepted that there is a threshold dose below which an effect will not occur.

Consequently, risk assessment for chemicals having noncarcinogenic effects usually involves determining the so-called "no observable effect level" (NOEL) from tests conducted with laboratory animals or occasionally with people. It is important to recognize that, since the NOEL is the highest dose tested at which no adverse effect was observed, it is a value that is determined experimentally. The NOEL constitutes a useful benchmark from which a variety of regulatory numbers are derived. One of these, the "acceptable daily intake" (ADI) or "reference dose" (RFD) is the estimated daily dose to which humans can be exposed for a lifetime without suffering any adverse effects; it is used routinely by the EPA in establishing HAs and other health-based standards for drinking water contaminants. The RFD is derived simply by dividing the NOEL by a "safety factor" of 10, 100 or 1,000 intended to account for possible differences between the test species and humans and for interindividual differences between people. The size of the "safety factor" is directly proportional to the degree of uncertainty in the data; in fact, it would be more appropriate to call it an "uncertainty factor." For noncarcinogenic chemicals the MCLG is usually set at a level corresponding to a percentage of the RFD.

In summary, there is always a very substantial margin of safety incorporated into EPA's health advisories and standards for chemicals causing noncarcinogenic adverse effects.

The data in Table 2 for nine pesticides found with some frequency in ground-water, clearly show that the concentrations at which most occur are usually well below the EPA's lifetime HAs. Only in the cases of the insecticides aldicarb and carbofuran do the upper limits of the concentration ranges exceed the HAs and these levels occur only in a very small percentage of the contaminated wells. To date, there have been no reported acute adverse effects on human health associated with pesticide residues occurring in ground water noncarcinogenic adverse effects.

Table 2.
Groundwater concentrations of selected pesticides having the potential for
causing noncarcinogenic effects¹

Chemical	Use ²	Concentration range (ppb) ³	Lifetime Health Advisory (ppb) ⁴
Atrazine	H	0.3 - 3	3
Cyanazine	H	0.1 - 1	8.8
Metribuzin	H	1 - 4.3	175
Metolachlor	H	0.1 - 0.4	10
Propachlor	H	0.2 - 0.5	92
Aldicarb	I,N	1 - 50	10
Oxamyl	I,N	5 - 65	175
Carbofuran	I,N	1 - 50	36
Fonofos	I	0.1	14

¹Several of these materials are also considered by the
EPA to be possible animal/human carcinogens.

²H = Herbicide, I = Insecticide, N = Nematicide

³From EPA 1987

⁴From respective EPA health advisories

Carcinogenic Chemicals

Assessing the likely occurrence of chronic health effects, particularly cancer, presents a quite different and certainly more difficult problem. Here, instead of measuring obvious adverse effects resulting from high doses over short periods of time, the object is to detect, in populations, the occurrence of low probability events (i.e. tumor formation) resulting from exposure to very low doses over long periods of time -- usually a lifetime.

The fundamental problem that exists in cancer risk assessment (Wilkinson 1986) is the inescapable need to extrapolate from effects observed under one set of conditions in the laboratory (i.e. rodents exposed to high doses) to predict those likely to occur under another set of conditions in the real world (i.e. people exposed intermittently to very low doses). Short of conducting tests with impossibly large (>50,000) numbers of animals, there is just no way to measure carcinogenic effects occurring at the low doses relevant to human exposure. Consequently, it is common to use high doses of the test chemical (usually at or approaching the "maximum tolerated dose") and to assume that it is possible to extrapolate from the effects observed at such doses to predict those likely to occur at the low doses of interest.

Regulatory philosophy continues to cling to the concept that, for carcinogens, there is no finite threshold below which an effect will not be observed. Consequently, while we have no idea about the shape of the dose-response curve at doses lower than those used in the experiment, low-dose effects can only be estimated by extrapolation through zero. This step of the risk assessment process, typically involving extrapolation over a dose range of four, five or six orders of magnitude (far greater than would be acceptable in most other areas of science) is accomplished by the use of several available mathematical models.

It should also be emphasized that the cancer risk estimates generated by the EPA are always upper bound (95 percent confidence limit) estimates, not "most likely" estimates, of risk. They are

highly conservative values based on worst-case estimates derived from the most sensitive test species using worst-case assumptions of human exposure. The real risks are always very much lower than the upper bound values stated, and in most cases could easily approach zero. The result of all this is that what appear to be very precise estimates of human cancer risk can vary by many orders of magnitude depending on the models and assumptions through which they were obtained. It is generally agreed that the estimates generated by the EPA are always highly conservative, so much so that, in most cases, it is unlikely that they have much in common with the real world.

SETTING THE STANDARDS

In generating MCLGs, MCLs and HAs for chemicals occurring in drinking water the EPA places a material into one of three major categories:

- Category I -- chemicals classified by the EPA as either "human carcinogens" (EPA Group A) or "probable human carcinogens" (EPA Group B1 or B2);
- Category II -- chemicals considered by the EPA to exhibit "equivocal evidence of carcinogenicity" and thus classified as "possible human carcinogens" (EPA Group C); and;
- Category III -- chemicals with "inadequate or no evidence of carcinogenicity in animals" (EPA Groups D and E).

As discussed already, MCLGs, MCLs and HAs for category III chemicals are all based on RFD values that are in turn obtained by the application of uncertainty factors to NOELS.

In contrast, MCLGs for Category I "non-threshold" chemicals have been set at zero because regulatory philosophy dictates that no "safe level" of exposure can be established. The MCLG is intended to reflect the long-term goal of the SDWA. Proposed MCL values for these chemicals reflect current technical feasibility (i.e. practical reality) and while the EPA sets no lifetime HA for a carcinogen, a water concentration calculated to cause a one in a million (10^{-6}) lifetime risk of cancer is usually provided. The latter suggests an attempt by the EPA to establish an unofficial de minimis risk value, a regulatory benchmark that might be used to separate what is considered an insignificant and presumably acceptable level of risk from one that is considered significant and therefore unacceptable. Unfortunately, since MCLGs for carcinogens are zero, and since MCLs presumably must be reduced toward zero whenever technical feasibility allows, the SDWA rejects the notion that any finite level of risk can be considered insignificant.

Regulatory standards for Category II chemicals may be established following either "threshold" or "non-threshold" methods depending on a judgement call on the part of the regulator.

PUBLIC MISCONCEPTIONS OF CANCER

The conservative cancer risk estimates promulgated by the EPA are usually taken at face value by non-scientists and the media and have had an enormous impact on the public's perception of cancer. Cancer, of course, holds a special kind of dread for most of us and, to be sure, current figures suggest that it will eventually claim the life of one in every four or five of us. There is widespread public belief, however, that:

- a) we are in the midst of a cancer epidemic in this country and
- b) this is due primarily to exposure to synthetic chemicals.

It should be stated emphatically that with the notable exception of lung cancer, deaths from which have tripled since 1950, and skin cancer that has also gone up substantially, death rates from most forms of human cancer have stayed more or less constant or increased very slightly over the last 35 years or so; mortality from some, such as stomach and rectal cancer has markedly decreased. If lung cancer is excluded, there has been a steady decline in total cancer mortality since 1950. Consequently, with the one real exception of lung cancer, known to be due mainly to smoking cigarettes, there is no epidemic of human cancer in the U.S.

Studies by the most respected epidemiologists, toxicologists and cancer experts show that, in fact, only a relatively small fraction of human cancers can be attributed to synthetic chemicals as shown in Table 3. Even in the most highly industrialized countries, occupational exposure is considered to account for no more than about 5%, and the total contribution of environmental pollution is estimated to be only 1-2%.

In contrast, cigarette smoking alone accounts for some 30% of all male cancer (it has also passed breast cancer as the major killer in women) and the consumption of alcohol and sexual behavior may cause an additional 10%. It is estimated that factors associated with diet may be responsible for about 35% of all human cancer.

Dr. Bruce Ames of the University of California in Berkeley believes that 99.99% of the carcinogens that most people ingest are from natural sources (in our food) or from what he calls traditional sources (cigarettes, alcohol and chemicals formed during cooking) (Ames et al. 1987). In other words, of the total carcinogen load that most of us are exposed to via food and water, about 10,000 times more comes from naturally-occurring materials than from those of synthetic origin.

So why do we continue to worry so much about the potential carcinogenic effects of synthetic chemicals such as pesticides?

Table 3.
Causative factors in human cancer¹.

Factor or class of factors	Percent cancer deaths
Tobacco (mainly cigarette smoking)	30
Alcohol and sexual behavior	10
Diet	35
Occupation	5
Environmental Pollution	2
Geophysical (e.g. radiation)	3
Infection	10
Miscellaneous (unknown)	5

¹Modified from Doll and Peto 1981.

Risk Perception and Acceptance

The answer is complex and relates, in part, to the way in which we perceive and respond to the different kinds of risk that we all face every day. A major factor relating to what level of risk we are willing to accept is the degree of control that we, as individuals, feel we can exert over the situation. Thus, we willingly accept a lot of quite large risks over which we feel we have control, but are not willing to accept even very small risks imposed on us by someone else. A sentiment often expressed is "Why should I have to accept a 1 in a million risk of cancer from drinking water containing this chemical?" This attitude is certainly exacerbated by, if not an inevitable consequence of, a regulatory policy that categorically denies the existence of a safe level of exposure for carcinogens; a carcinogen is a carcinogen at any concentration.

The Need for De Minimis

Such a policy dictates that, in the real world, where traces of synthetic chemicals classified as carcinogens will be detected in drinking water with increasing frequency, regulators must make decisions as to whether to close down a particular source (often a decision with very serious economic ramifications) or whether to wrestle with the problem of what constitutes an acceptable level of risk. Regardless of whether a theoretical threshold exists for carcinogens, most scientists and regulators agree that there are practical thresholds below which risks, if any, are quite negligible. It is essential, therefore, that some de minimis level of risk, acceptable to the public, be adopted by the EPA (either unofficially or officially through an amendment to the SDWA) as a "virtually safe dose." Dr. Ames has suggested that an appropriate de minimis level of risk for carcinogen intake from water might be that equivalent to the chloroform present in ordinary chlorinated tap water. This seems a very sensible suggestion that most people should be able to accept. Thus, although chloroform is classified as a carcinogen by the EPA, the Agency allows up to 100 ppb chloroform in drinking water, a concentration that, on the basis of a daily intake of two liters of water per day, is estimated to cause a lifetime cancer risk of 1.7×10^{-5} (almost 2 in 100,000).

Table 4 shows how this level of risk compares with the risks associated with consuming two liters of water containing the pesticides ethylene dibromide (EDB) and dibromochloropropane (DBCP) at the levels they have been reported, and from drinking water containing the EPA limit of trichloroethylene (5 ppb).

Table 4.
Estimated risks associated with selected carcinogens in drinking water.

Chemical	Concentration in water (ppb)	Lifetime cancer risk
Chloroform	100 ¹	1.7×10^{-5} ²
Trichlorethylene	5 ¹	1.6×10^{-6} ³
EDB	0.05 - 20 ⁴	1.0×10^{-6} - 3×10^{-4} ⁵
DBCP	0.02 - 20 ⁴	0.8×10^{-8} - 8×10^{-6} ⁵

¹ EPA MCL;

² Calculated from a q^* value of 6.1×10^{-3} (mg/kg/day)⁻¹;

³ Calculated from a q^* value of 1.1×10^{-2} (mg/kg/day)⁻¹;

⁴ Range of concentrations found in groundwater;

⁵ Taken from EPA Health Advisories.

Dr. Ames has pointed out how irrational we are in our approach to regulating chemicals in water. According to his calculations (similar to these shown in table 4), of the wells closed down in Silicon Valley, CA and Woburn, MA because of their presumed carcinogenic hazard from trichloroethylene, very few constituted a greater hazard than ordinary chlorinated tap water. Water from even the most contaminated wells was still about 1,000-fold less hazardous than an equal volume of cola that contains formaldehyde or beer containing formaldehyde and alcohol. Indeed, according to Dr. Ames:

"The carcinogens and pesticide residues currently being found in California water supplies, such as Silicon Valley, are present in such extraordinarily small amounts that, except in rare cases, they are trivial relative to the background of carcinogens in nature. Therefore, I am convinced that such water pollution is irrelevant as a cause of human cancer."

Relative Risk

While many people may not agree fully with Dr. Ames, it is evident that we are spending a great deal of time, effort and money in attempting to identify and regulate chemicals, especially those classified as carcinogens, occurring at very small concentrations in our food, air and water. We become involved in ferocious debate about how to deal with risks considerably lower than one in a million. Perhaps one reason for this is that most people find it difficult to place risks of this magnitude into proper perspective and compare them with other more "familiar" risks encountered each day. Table 5 clearly shows the relatively large risks of death associated with many familiar occurrences and it can be seen that even bee stings are associated with a 14 in a million lifetime risk of death.

Work-related deaths in various occupations are even more startling, with mining, construction, transportation and agriculture being associated with risks of death of about 19, 11, 8 and 8 per 1,000, respectively. These values should serve to place in better perspective the kinds of chemical risks about which we are currently so much concerned. Interestingly enough, however, most people seem remarkably unimpressed with figures of this type and remain concerned about that one in a million cancer risk. Communication continues to be a serious problem and hard facts do little to change an emotional conviction. In recent years, Dr. Ames has taken another approach, comparing the risks associated with potential synthetic carcinogens against those of naturally occurring materials considered to have carcinogenic potential.

Table 5.
Lifetime risk of death from selected occurrences.

Occurrence	Lifetime death rate (per million)
Motor vehicle accident	13,720
Home accidents	7,700
Falls	3,430
Drowning	1,680
Fires, burns	1,400
Electrocution	370
Tornado	40
Bee sting	14

With respect to pesticide residues, for example, Dr. Ames has pointed out that the potential risk (EPA estimate) from the pre-1983 daily dietary intake of EDB in grain products was some 75-fold lower than that of a peanut butter sandwich (aflatoxin) and 200-fold less than that of a single raw mushroom (hydrazines). He has calculated that the U.S. population consumes approximately 46 g of potentially carcinogenic pesticide residues each day in food and water. By comparison, a single cup of coffee contains about 500 g of potentially carcinogenic residues (methyl glyoxal, hydrogen peroxide, etc.).

FUTURE DIRECTIONS

It is not the objective of this paper to state that there are not some situations in which chemicals may pose a serious threat to human health. Clearly there are, and we must always keep a watchful eye to identify and/or remedy such situations. On the other hand, both as individuals and collectively as a society, it is important for us to place into better perspective the potential health risks associated with traces of synthetic chemicals in our food and water. At the present time we are unable to distinguish trivial risks from those of a more serious nature and we greet each new piece of "bad news" with the knee-jerk response that once again the sky is falling.

Both individual and societal responses to continued bad news ranges from excessive anxiety to defensive indifference. The public's health can be seriously compromised by continual worry and stress and with so many "scares" people tend to become cynical and resigned to their inevitable fate. If everything causes cancer there is little incentive to try to resolve more serious "fixable" problems such as smoking. Also, the constant cry of "wolf" may dull our ability to respond when a real crisis comes along.

Public perceptions of risk also play a major role in policy and regulatory decisions at the state and national level. There is no question that our regulators and legislators are influenced to a significant extent by public opinion and may be pressured into making costly wrong decisions if public concern is misdirected. We must never underestimate the importance of risk communication to the public and we must be careful to get our priorities straight and not divert attention and dollars along unproductive pathways.

Perhaps, ultimately, we can develop a more rational societal attitude that will allow us to make informed, intelligent decisions based on the scientific evidence available. Perhaps we will even learn to accept as commonplace a few risks that today remain a source of considerable concern.

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DISCUSSION OF KEYNOTE ADDRESS - CHEMICALS IN WATER: GETTING A HANDLE ON HEALTH RISKS BY C.F. WILKINSON

Ron Sims¹, Presiding
David Stevens², Recorder

TITLE

Chemicals in Water: Getting a Handle on Health Risks by C.F. Wilkinson

SPECIFIC QUESTIONS AND COMMENTS

Note:

Following the presentation on "Chemicals in Water: Getting a Handle on Risks" by Dr. Chris F. Wilkinson, a lively discussion ensued centering on public perception of risks and effective risk communication.

Comment: (C. Wilkinson, Cornell University, Ithaca, New York) We must set health priorities so that limited funds available to address technological problems are used wisely to solve our most pressing problems that do present high levels of risk to human health. The setting of priorities should be based as much as possible on scientific facts; however, public opinion and public perception of risk concerning hazardous substances in the environment is driven by an obsession, on the part of the American people, with cancer. Resulting emotionalism makes it difficult to communicate the significance of risks posed by the presence of extremely low concentrations of hazardous substances in water supplies. Special interest groups that play a "watchdog" role over the U.S. Environmental Protection Agency (EPA) sometimes force EPA to develop regulations that are more strict than the degree of risk would dictate.

Comment: (Audience) We must also consider the trade-offs made when minimizing or eliminating one type of risk, only to replace that risk with another risk due to replacement activity to achieve a similar goal. Also, we can only use methods based on the best scientific information available at the time and can never be sure of what is "absolutely" safe. However, a more conservative approach than that of Dr. Wilkinson's to release chemicals in the environment, would be prudent because of the uncertainty in long-term protection of human health.

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POLLUTION OF WATER FROM AGRICULTURE: SOCIOECONOMIC AND POLITICAL ISSUES

Pierre Crosson¹

ABSTRACT

Policies to deal with agricultural nonpoint-source water pollution must consider issues of both economic efficiency and social equity. The joint efforts of natural scientists and social scientists are needed to effectively address this vital task. These issues are discussed in the context of U.S. experience with surface water pollution from sediment and associated agricultural chemicals.

INTRODUCTION

The discussion deals with socioeconomic and political issues presented by nonpoint-source water pollution which I believe are common to all countries. However, the specifics of these issues are discussed with reference to the United States, the only country I know much about in these respects.

SOURCES AND COSTS OF DAMAGE

Sediment, pesticides, fertilizers, animal wastes, salt, and other material carried in irrigation return flows have long been recognized as the main threats from agriculture to water quality. Only recently, however, do we have estimates for the United States suggesting the relative importance of the threats. Clark and associates at the Conservation Foundation (1985) estimated annual sediment damages to be between \$4 billion and \$16 billion, with a "best guess" estimate of about \$8 billion (1985 prices). Pimentel and colleagues at Cornell (1980) estimated annual pesticide damages--of all sorts, including human illnesses and deaths, not just impaired water quality--to be some \$800 million (probably prices of the 1970s). Both of these estimates leave out various costs, so in that sense they set lower bounds. They suggest that, measured by the economic cost of the damage, sediment is a far more serious threat to water quality than pesticides.

Problems of salinity damage associated with irrigation in the United States are confined for the most part to the lower Colorado basin, parts of the Imperial and San Joaquin valleys of California, and parts of the Rio Grande basin. Drawing on a variety of studies, Clark and associates (1985) estimate the cost of the damage in reduced agricultural production at \$3 million to \$34 million annually, with a "best guess" estimate of \$25 million. These estimates are in 1980 prices. In 1985 prices they would be a quarter to a third higher. Saline water can also increase treatment costs of water delivered to municipal and industrial users. Comprehensive estimates of these nonagricultural damages are not available, but even if they are an order of magnitude higher than the costs to agriculture, total salinity costs would be no more than half the costs of pesticides estimated by Pimentel and associates, and an order of magnitude less than the minimum estimate of sediment damage by Clark et al.

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Fertilizers and animal wastes carried in runoff to surface waters or which percolate to groundwater impose a variety of damages, e.g., eutrophication of lakes, reservoirs and estuaries, and impaired human and animal health, although instances of human health impairment are rare. I have seen no estimates for the United States of the economic costs of these damages comparable to those for sediment, pesticides, and salinity in irrigation return flow. But it appears to me that the public discussion of water pollution issues gives less attention to damages from fertilizers and animal wastes than to those from pesticides. The distribution of public attention is not a sure indicator of the relative importance of the various threats but neither, I believe, is it irrelevant. On the limited present evidence I conclude that in the national perspective taken here sediment is the greatest threat to water quality and that fertilizers and animal wastes are much lesser, if not the least, threats.

By now some of you may be beginning to feel uneasy about the reliance here on economic costs as the measure of water quality damage caused by agricultural pollutants. Can dollar values capture the full costs of these damages? In particular, can human deaths and illnesses be adequately expressed in an economic calculus, or the social cost of impaired habitat, as in the famous case of the Kesterson Wildlife Refuge in California?

The questions reflect a philosophical, and perhaps religious, view of the value of human life and of the sanctity of the natural system which we humans jointly share with all other life forms. I sympathize with this view, and indeed share it to some extent. But while the view tempers, it does not negate the importance of economics in trying to establish priorities among the various threats of agricultural pollutants to water quality. If as a society we are to act sensibly to meet these threats, we must make judgments about their relative importance. Measures of economic cost help us to do this. No one with an expansive sense of the values at stake and knowledgeable about political processes would argue that economic measures of cost could be, or should be, the sole basis for these judgments. But neither would such a person deny the relevance of the measures as rough guides to pollution control policy. Economics is far from being all there is to it, but it counts.

NATURE OF THE POLICY ISSUES

However we might rank the various nonpoint sources of damage to water quality--as noted, for the U.S. I rank sediment first--in what sense do the damages pose policy issues? What is it about the damages that justifies public intervention to reduce them?

Economic Efficiency

Economists generally respond to this question along two lines. One is that if by spending an additional dollar to reduce the damage we can get more than a dollar's worth of damage reduction, then failure to spend the additional dollar would be an inefficient use of society's resources.

There are two things to be said about this efficiency argument. One is that the mere existence of pollution damage is not in itself evidence of inefficiency. Permitting continued pollution is socially inefficient only if the incremental cost of pollution reduction is less than the incremental cost of pollution damage. Since for most pollutants the incremental cost of reducing them rises as the total amount reduced increases, and the social value of additional damage reduction is constant or decreasing, then in the general case reducing pollution damage to zero would be inefficient. For example, reducing sediment pollution of water to zero surely would cost far more than the resulting gain in economic, environmental and any other social value.

The second thing to be said about the efficiency argument is that while the mere existence of pollution damage is not sufficient evidence of inefficiency, in many if not most cases the damage in fact is inefficient, if there are no policies in place to reduce it. That is to say, in these cases the social incremental cost of reducing pollution damage likely is less than the social incremental cost of the damage. If this seems to contradict the first statement about efficiency, bear with me. The basis for the second statement is that since in the cases specified, the polluter does not pay the cost of the pollution damage, he will treat the cost as zero. Since the cost of reducing the damage is greater than zero, the polluter will not invest in damage reduction. The result is efficient for the polluter, but not for society.

The implication of these two statements about efficiency is that although the mere existence of pollution damage is not a sufficient reason for policies to reduce it, the institutional conditions under which pollution occurs frequently cause private investment in pollution control to be less than the socially efficient amount. There is a presumption, therefore, that in the absence of control policies, the amount of pollution is socially inefficient. Whether the presumption is justified in particular cases, however, cannot be determined without investigation of the circumstances of those cases. Moreover, in those cases where control policies can be justified on efficiency grounds, the socially optimal amount of control will seldom if ever carry pollution damage to zero.

Social Equity

Apart from efficiency, pollution control policies are also justified on equity grounds. The basic equity argument is simple--deceptively so. The polluter causes the damage, but does not pay for it. Someone else does, either in the polluter's generation or in some subsequent generation. Most of us can agree that such situations raise equity issues. And while most of us also would agree that no society can ever hope to achieve complete equity within and across generations--life, as President Kennedy once remarked, is unfair--we nevertheless believe that no society can be indifferent to equity. Indeed, I think it fair to say that public policy, whether for water pollution control or anything else, is driven far more strongly by equity considerations than by concerns about economic efficiency.

Achieving equity in public policies, or even knowing it when we see it, is inherently more difficult than achieving efficiency. In principle we have an objective standard for efficiency in pollution control policy: we exert control to the point where the incremental cost of control equals the incremental value of the reduction in pollution damage. As a practical matter, of course, we find it difficult to achieve the standard, but at least we can define it unambiguously.

This is not the case with equity. Equity is a far more complex concept than efficiency. Different societies at any given time will have different standards of equitable arrangements among their members. Witness the differences between present day fundamentalist Moslem societies and western societies about the social position of women. And standards of equity in any given society will change over time. Witness the United States. Only a little over 100 years ago most people in this country evidently believed that slavery in the Southern states was consistent with generally-accepted canons of equity in American life.

Because equity is such a complex concept, generally acceptable objective standards of it are not available, probably not even in principle. In all societies, there are simply too many instances in which my equity is your inequity. This is not to say that equity is wholly a subjective concept, but that on many, if not most social issues, any consensus about equity is likely to be subject to numerous reservations, qualifications, and nuances of understanding, some explicitly stated, some only implicit. Consequently, achieving policies that satisfy everyone's sense of equity is probably impossible. The problem is compounded when we seek--as we should--to make those policies also meet standards of efficiency.

An Example

A hypothetical example will help to illustrate the problems of devising policies to control nonpoint-source pollution of water which meet criteria of both equity and efficiency. Suppose I have built an elegant, and profitable, recreational facility along a stretch of sparkling clear river. Then one day upstream from me you decide to switch from pasture to corn and soybeans and begin to dump massive amounts of sediment in the river. The value of my facility is severely diminished. However, suppose that the loss of value to me is less than what it would cost you to control the dumping of sediment. Assuming away all problems of market imperfections, the situation represents a socially efficient use of resources. It follows that public intervention to require that you quit dumping on me could not be justified on efficiency grounds.

But is the situation equitable? I think not. You think it is, if you think about it at all. Since I have no property in your stretch of the river I cannot charge you for using it as a dump for your sediment. The usual market mechanism for exacting compensation for cost of services rendered, therefore, is not open to me. If I am to be compensated I must seek it through other means: friendly persuasion, or, failing that, the courts, possibly the political process, or, if this were an earlier time, perhaps through more direct and forceful measures.

The point is that I am wholly unimpressed by the fact that your dumping on me reflects a socially efficient use of resources. My sense of equity is offended and so far as I am concerned that is sufficient to make the situation between us a policy issue. If there are enough such situations around the country, those responsible for water pollution control policy will likely come in time to share my perception. Of course it does not necessarily follow that whatever policies are adopted to deal with such situations will be to my liking. The fact that your dumping is socially efficient will, or should, weigh against me, although it will not, or should not, necessarily be decisive.

Another Example

Now consider a superficially similar but in important respects different situation. You and neighboring farmers have long engaged in corn and soybean production on sloping, deep loess soils. In the process, you have dumped several million tons of soil each year into tributary streams for ultimate delivery out of the watershed. Despite the high concentration of suspended sediment and associated chemicals in the water at the watershed mouth no one complained because little use was made of the water at that point. The social cost of the poor water quality was nil. Indeed, it is not even clear that the words "poor water quality" mean anything if the water has no social value, whether clean or dirty.

Now suppose that the community at the watershed mouth grows to the point that the aquifer on which it had always depended for its water supply no longer will suffice. The only source of additional water is the dirty stream running through the community, but the water must be treated to bring it to potable standards. Now the cost of the poor water quality is high. A study done by a consulting firm shows that the most efficient way to clean up the water is to control erosion at the source--that is, on your land and that of your neighbors--rather than to treat the water at the watershed mouth. Moreover, you and your neighbors clearly are responsible for the dirt and related pollutants in the water. Thus efficiency indicates erosion control on your land as the clean-up instrument, and equity, say the community leaders, indicates that you and your farming neighbors should pay the cost of control.

You might readily accept the efficiency argument for erosion control, but wholly reject the equity argument that you and your neighbors should pay for it. You and your neighbors have "always"--that is, for many years--dumped soil and chemicals in the local streams, with no complaint from anyone. You claim no formal property right in the streams, but you argue that long usage, unopposed downstream, has established an informal right, which now would be rudely

violated. You and your neighbors, after all, are not responsible for the growth which produced the community's water supply problem. They caused the problem, not you. Let them pay for solving it.

These hypothetical cases serve to highlight several points:

- (1) Efficiency counts in water pollution control policy, but equity probably counts even more.
- (2) Most people can accept the economic efficiency criterion for policy and agree on what it means because it is simply a technical statement of a widely held, and understood, moral precept: waste not. Accordingly, given all the relevant data, people can agree reasonably well on what to do when commanded, "Be efficient."
- (3) Similar agreement on the equity criterion for policy is much more difficult because there is an inherently subjective element in judgments of equity. Consequently, agreement on how to respond to the command "Be equitable" is harder to achieve, whatever the amount of data provided.
- (4) Both the efficiency and the equity issues raised by nonpoint-source pollution of water are owed in large measure to the absence of clearly defined property rights in the water. If I owned the stretch of river between you and me I would charge you a fee for using it as a dump for your sediment, the fee being not less than the cost to me of your dumping and not greater than the cost to you of not dumping. If these conditions for the fee were met, you would dump and pay me the fee. If they were not, you would not dump and would pay the cost in reduced income. In either case, the social cost of using the water as a dump for your sediment would be fully reflected in both your calculations and mine. The resulting use of our resources--mine the river and yours the land--would be efficient for both of us and for society as a whole. And, so long as my property right in the river were in fact clear and legal, you would have no grounds in equity to complain about paying the fee.

If you had clear title to the intervening stretch of river, you would charge me a fee for using it as the site of my recreational facility. The fee would be not less than the cost to you of not dumping, and not more than the value to me of the water for recreational uses. Again, if these conditions were met, our respective uses of the land and water would be efficient for each of us and for society as a whole. And I would have no grounds for disputing your right to charge me a fee for using your water.

SEEKING POLICY SOLUTIONS

I hope I have convinced you that those responsible for water pollution control policy must deal with a complex tangle of efficiency and equity issues. I now am going to argue that the more information policy makers have about the efficiency issue, the more readily they can untangle the tangle. The argument rests on several propositions:

- (1) Often--usually?--policy makers lack the information needed to specify what an efficient solution to a water quality problem would look like. On the assumption that efficiency is an important objective of water quality policy, providing the missing information obviously would improve the policy process.
- (2) Vested interests who feel threatened by new policies seldom state their opposition to the policies, or their defense of old ones, on equity grounds, recognizing that this would be

too transparently self-serving. They are more likely to argue that the new policies are undesirable because they would be inefficient. More information about what a truly efficient solution would look like helps to unveil these vested interest arguments against the solution.

- (3) Better information about the efficiency aspects of a water quality issue often can narrow differences about the equity aspects, thus easing the policy problem. The differences about equity dividing you and neighboring farmers from the downstream community about who should pay for the cost of providing clean water to the community perhaps could be reduced if analysis showed that without significant sacrifice of income by you and your neighbors, conservation tillage would most efficiently achieve the needed reduction in sediment delivered downstream.

Of course, I do not argue that better understanding of the efficiency aspects of water pollution problems will of itself resolve all policy issues. Even complete understanding of these aspects no doubt would leave some differences between contending parties about equity aspects. And the power of vested interests to resist public scrutiny should never be underestimated. Nevertheless, so long as efficiency counts in water pollution control policy, more knowledge about the characteristics of efficient solutions will promote the policy process.

CONTROL OF SEDIMENT DAMAGE: A CASE IN POINT

It has long been recognized in the U.S. that by volume sediment is the main pollutant of the nation's surface waters. Since the work of Clark and associates at the Conservation Foundation (1985) showing that costs of sediment damage run to billions of dollars annually, sediment control has emerged in this country as a major, if not the major issue in surface water pollution control policy.

The 1972 Clean Water Act Amendments gave the U.S. Environmental Protection Agency responsibility for control of nonpoint-source water pollution. Under section 208 of the Act the EPA delegated this responsibility to the states, requiring each of them to submit plans to achieve the water quality objectives of the Act. Continued state planning to this end is mandated under section 319 of the Clean Water Act of 1987.

The state 208 plans relied heavily on erosion-control practices developed by the Soil Conservation Service (SCS) of the U.S. Department of Agriculture (USDA). It appears that under Section 319 of the 1987 Act, erosion reduction will remain the principal instrument for control of agricultural nonpoint-source pollution of surface water.

A study by Smith, et al. reported in *Science* (1987), suggests that as recently as 1981 the state planning efforts had had little effect in cleaning up the nation's surface waters. The study found that between 1974 and 1981 there was no trend in amounts of sediment and total phosphorus delivered, and nitrate concentrations actually increased.

This finding does not necessarily prove that the state 208 plans were ineffective. For reasons developed below, lags of several years, or even a decade, could easily occur between a reduction of erosion on the landscape and a related reduction in downstream deliveries of sediment and associated pollutants.

A study by Strohbehn and colleagues at the USDA's Economic Research Service (1986) raises a more fundamental question about erosion control to reduce agricultural nonpoint-source pollution. This study indicates that the cost of the USDA's erosion control programs exceeds the

benefits in reduced off-farm damages by a substantial margin. The average benefit-cost ratio for the programs remains less than one, even when the soil productivity benefits of reduced erosion are included in the calculation. Only on cropland with pre-control erosion rates in excess of about 45 metric tons per hectare, 4 times the "tolerable" rate, were the combined productivity-off-farm benefits greater than the costs of control, and even on that land there was some ambiguity in the results.

Taken at face value, the studies by Smith et al. (1987) and Strohbehn et al. (1986) indicate that erosion control programs have been ineffective in reducing deliveries of sediment and related pollutants to the nation's waters, and that it would be socially inefficient to spend more on the programs, despite the high cost of these pollutants in impaired water quality.

However, the studies should not be taken at face value, for several reasons. As already noted, delays would be expected between a reduction in erosion on the landscape and a related reduction in downstream deliveries of sediment and related pollutants. Moreover, the estimates by Strohbehn et al. of benefits of cropland erosion control may be low. The benefits are calculated as reductions in costs of sediment damage as estimated by Clark and associates at the Conservation Foundation. However, the estimates of Clark et al. do not include some costs that could be important, such as damage to ecological systems. Were reductions in these costs included, the benefit estimates of Strohbehn et al. likely would have been higher.

Strohbehn et al. (1986) found that cropland erosion control gave zero benefits in reduced damages to water-based recreation. This is a counter-intuitive result because the study by Clark et al. found that loss of recreation values was one of the most important kinds of sediment damage. The Strohbehn et al. result reflected the fact that they used a certain standard for ambient water quality to judge whether reductions of sediment and related pollutants improved quality. Even though pre-control erosion might be very high and the reduction in erosion and sediment delivered substantial, no improvement in water quality would occur unless the reduction passed the threshold set by the standard. This procedure is defensible, particularly with respect to nutrients in water. But the use of a threshold to measure improvements resulting from reductions in sediment delivered is arguable.

The threshold concept as used by Strohbehn et al. is even more questionable because their study focused only on cropland erosion control. Although per hectare erosion rates are relatively low on range, pasture, and forest land, so much land is in these uses that collectively they contribute 60 percent as much sheet and rill erosion as cropland. Consequently, even very large reductions in sediment delivered from cropland might not pass the threshold for judging improvement so long as erosion from range, pasture and forest land were unchecked.

Finally, it is important to note that much, if not most, sediment damage occurs in situations where property rights in the damaged water are not clear, or not readily enforceable. This supports a presumption that the costs of the damage are inefficiently high; and for the reasons given, I do not consider the Strohbehn et al. findings strong enough to override the presumption. Moreover, even if those findings were conclusive that existing levels of sediment damage are not socially inefficient, the institutional conditions under which the damage occurs suggest the damage raises equity issues.

Thus, I consider the question of whether we in the U.S. should spend more to reduce off-farm damages of sediment and related pollutants as still open, on both efficiency and equity grounds. However much we spend, there are strong efficiency arguments for spending it differently. The first argument is based directly on the finding by Strohbehn et al. that the combined productivity/off-farm per-hectare benefits of erosion control increased steeply with the amount of pre-control erosion per hectare. Of the 6.7 million hectares of cropland considered by Strohbehn et al., 38 percent had pre-control erosion rates less than the "tolerable" amount. The

total benefits of erosion control on this land were \$8.20 per hectare. Thirteen percent of the land had pre-control erosion rates in excess of 4 times the "tolerable" rate, but the benefits of control on this land were \$124.50 per hectare. Thus the benefits of erosion control on land which in the absence of control would erode at 4 times the "tolerable" amount were 15 times greater than benefits on land with pre-control erosion less than the tolerable amount. This is strong evidence that however much we in the U.S. spend on soil conservation, we could spend it much more efficiently if we concentrated on the most highly erosive land.

Incidentally, the Strohbehn et al. study also showed that the off-farm benefits of cropland erosion control were 75 percent greater than the productivity benefits, suggesting that, if total spending on soil conservation is fixed, efficiency would be served by spending less to protect soil productivity and more to reduce off-farm sediment damage.

The Conservation Reserve Program (CRP) is encouraging evidence that the USDA, under mandate from the Congress, is beginning to shift erosion control toward more highly erosive land. This is a step in the right direction. The step is limited, however, because it rests on the fundamental assumption that the most efficient way to reduce off-farm damage of sediment and related pollutants is to reduce on-farm erosion. Two sorts of evidence suggest strongly that this is not so. One sort is from studies comparing the effectiveness of erosion control and sediment control in reducing edge-of-field deliveries of sediment and related pollutants. The other sort is studies of the relationship between on-farm erosion control and downstream sediment delivery.

The first sort of study is by Smith et al. (1979) and reports research on the effectiveness of various on-farm erosion control practices in reducing sediment delivery to a stream at the edge of the field. The traditional approach, for example in the study by Strohbehn et al. (1986), implicitly assumes that the effectiveness of erosion control practices in reducing edge-of-field deliveries of sediment is proportional to their effectiveness in reducing erosion. Smith et al. (1979) found this not to be so, i.e. two fields identical in all other respects, including crops grown, would generate the same amount of erosion but would deliver different amounts of sediment to the edge of the field, depending on their position relative to the edge. Accordingly, erosion control practices which have identical costs per ton of erosion reduction can have quite different costs per ton of reduced edge-of-field sediment delivery. It follows that, in general, a plan designed to achieve the most efficient reduction in sediment delivered from the farm will not be the same as a plan to most efficiently reduce erosion on the farm.

The second sort of study casting doubt on on-farm erosion control as the most efficient way of reducing sediment delivery is based on recognition of the fact of often large spatial and temporal discontinuities between the occurrence of erosion on the farm and the occurrence of sediment damage downstream. In a seminal article Wolman (1977) noted that the relationship between on-farm erosion as measured by the Universal Soil Loss Equation (USLE) and the amount of sediment delivered to downstream points is tenuous and ill-understood. Walling (1983), Campbell (1985), Baker et al. (1985), and other researchers have come to the same conclusion. A major reason for this is that the USLE measures average annual erosion over a period of years, while sediment delivery is mainly driven by episodic storm events. The fact of long-term storage of sediment in various parts of watersheds, demonstrated by Trimble in the southern Piedmont (1975), Trimble and Lund (1982) in Coon Creek, Wisconsin, and by other researchers elsewhere, also is of prime importance.

The studies briefly reviewed provide strong arguments on efficiency grounds for rethinking the traditional policy of using on-farm erosion control to reduce off-farm damages of sediment and associated pollutants. These arguments can be summed up in two statements:

- (1) To the extent that on-farm land management remains the focus of policy, attention should shift from reducing erosion to reducing edge-of-field deliveries of sediment.

- (2) The focus on on-farm land management needs reconsideration. The spatial and temporal discontinuities in the relationship between on-farm erosion and downstream sediment delivery suggest that under many circumstances, sediment damage may be more efficiently reduced by controlling the sediment at or close to the point of damage than by controlling erosion on the farm upstream.

The point of departure for these statements is that where agricultural nonpoint pollution of surface water is the issue, the policy objective is reduction in sediment damage, not reduction of erosion. If the reduction in erosion were always proportional to the reduction in sediment damage, then the claim of erosion control as the favored policy instrument would be strong. But it is precisely the lack of such proportionality which suggests the policy shift, on efficiency grounds, to sediment management instead of erosion control.

Recognition of the spatial and temporal discontinuities between on-farm erosion and downstream sediment damage also has important equity implications. In terms of an earlier example, the downstream community likely would have great difficulty assigning responsibility among you and your neighbors for the sediment and related pollutants which foul the river flowing through the community. It would not be fair to assume that you were responsible in proportion to the amount of current erosion from your respective farms. Moreover, much of the sediment now delivered to the community may have originated years ago on land which then was under different ownership. You could not equitably be held responsible for that.

If equity requires that the polluter should pay--and as the earlier examples show, this may be an ambiguous standard of equity--then in such situations equitable solutions to the water quality problem would always be elusive. Would better information about an efficient solution to the problem provide a way around the equity issue? I think that in many instances it would. Returning to the example, suppose that analysis by that consulting firm shows that sediment stored in the watershed is so large relative to annual erosion on your farm and those of your neighbors that even if you all reduced erosion to well within tolerable limits, sediment delivered to the downstream community would remain high for a decade or more. Accordingly, the efficient solution to the community's water-quality problem would be to build a water treatment plant at the watershed mouth. The equity question is who should pay for it. Since the analysis supporting the efficient solution shows little connection between the community's polluted water and the current farming practices of you and your neighbors, and that moreover much of the stored sediment originated years ago on farmland now under different ownership, the community's argument that you and your neighbors should pay for the water treatment plant is weak. At least it is weaker than it would be if the efficiency analysis had not been done, for without the analysis the community could plausibly argue that (a) since sediment in its water is the problem and (b) you and your neighbors generate lots of erosion; therefore, (c) you and they must be responsible and should pay.

There clearly can be no guarantee that knowledge of the efficient solutions to these problems will also settle the equity issues the problems present. But no guarantee is claimed. My argument is the more modest one that better knowledge of the efficient solution could, in many instances, narrow the bounds of the dispute about equity.

The spatial and temporal discontinuities between landscape erosion and downstream sediment damage also have implications for the institutional forms best suited to management of damage control policies. The fact that in many instances efficient policies may call for some combination of landscape erosion control and downstream sediment management, and in some cases only the latter, suggests the value of institutions which can function across entire watersheds. I suggest that for the U.S. this raises a question about the role of soil conservation districts (SCDs) in the management of agricultural nonpoint water pollution. The SCDs are agencies of the states operating, with few exceptions, at the county level. Many watersheds extend well beyond single

county lines. The ability of SCDs to efficiently manage sediment control programs in those watersheds is arguable. Institutions whose geographic jurisdiction encompasses the entire watershed might be more efficient. Moreover, SCDs are erosion-control oriented. Accordingly, their mode of operation is to encourage farmers to adopt erosion-reducing land management practices. Where the erosion problem is loss of soil productivity, this is entirely appropriate. But where the problem is downstream sediment damage, erosion control, for the reasons already discussed, often will not provide the efficient solution.

RELEVANCE FOR THIS SYMPOSIUM

If we are to make headway in dealing with problems of agricultural nonpoint pollution of surface water we must have far more information about the conditions for efficient solutions to these problems. There is an enormous opportunity here for fruitful collaboration between natural scientists and social scientists interested in water pollution. The social scientists have the expertise to study the economic and environmental costs of water pollution and to evaluate the economic, social and political characteristics of alternative technical and institutional measures to control the costs. The natural scientists, such as those of you at this symposium, have the expertise to study the processes which link farmers' management practices with the generation and transport, by land, water and air, of sediment and other pollutants to downstream points, and which determine the effect of the pollutants on water quality. If the common objective of both groups of scientists is to reduce agricultural nonpoint pollution, then neither group can do without the other. The social scientists cannot estimate the cost of damages and the benefits and costs of damage reduction alternatives without information about the processes linking pollutant generation, transport and water quality damage. And the natural scientists cannot efficiently organize their research aimed at damage reduction without information from the social scientists about which problems promise the highest economic and social payoff in damage reduction.

This symposium provides a most valuable state-of-the-art assessment of key natural science aspects of the generation, transport and fate of agricultural nonpoint sources of water pollution. The challenge now is for those of us in the social sciences to make the vital linkages with your work. Together there is much we can do to help protect and promote the public interest in clean water. If we fail to do this we will fall short in our responsibilities as scientists and as citizens. Let us not let that happen.

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DISCUSSION OF KEYNOTE ADDRESS - POLLUTION OF WATER FROM AGRICULTURE: SOCIOECONOMIC AND POLITICAL ISSUES BY PIERRE CROSSON

Jay Andersen¹, Presiding
Bruce Godfrey², Recorder

TITLE

Pollution of Water from Agriculture: Socioeconomic and Political Issues by Pierre Crosson

SPECIFIC QUESTIONS AND COMMENTS

Note:

There was some discussion concerning the use of lands that had been put into the Conservation Reserve Program (CRP). It was noted that these lands could not, in the short run (ten years), be put into crop production. However, the USDA had approved the harvesting of hay in 1988 from some CRP lands as a method of relieving pressure for feed in areas of severe drought. The question was raised whether this was not counterproductive to the purposes of the program.

Response: (P. Crosson, Resources for the Future, Washington, D.C.) This decision represents a trade-off between reducing soil erosion (no haying allowed) and high short-term costs being incurred by farmers in these areas. One of the alternatives is to find high-cost sources of feed that may be substituted for hay obtained from these lands.

Comment: (Audience) A program similar to CRP was instituted in Minnesota. This program has an acronym of RIM (Reinvestment in Minnesota). It allows these lands to be grazed. It is believed that the soil erosion losses are essentially equal to those lands that are not grazed and in RIM. However, no empirical information is available concerning this supposition.

Response: (P. Crosson) CRP lands represent a large-scale experiment that needs to be evaluated by researchers.

Comment: (R. Hartzog, Louisiana Department of Environmental Quality, Louisiana) The measure of losses associated with erosion is essentially a question of determining if resources have been damaged and what the value is of these resources. This is a major empirical problem for researchers.

The studies that have been conducted at Resources for the Future (RFF) in the area of water quality and recreation benefits, that were cited earlier by Dr. Crosson, have set the precedence for this work but much work remains to be accomplished.

Comment: (C. Rose, Griffith University, Australia) There is not very much information available concerning on-site erosion and its impact on productivity. There are some questions that need to be resolved concerning whether it is less expensive to prevent erosion on-site or to treat its effects downstream. Some of the work that has been done in Australia has provided some empirical estimates for shallow soils and productivity losses. This work suggests that it is less costly to control erosion on site using agronomic tools than it is to treat the effects downstream.

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Response: (P. Crosson) Much of the work that has been done in the U.S. suggests that with technological improvements, the loss of on-site productivity is generally insignificant -- particularly on sites having deep soils. If on-site productivity losses are significant, it will generally be less expensive to control erosion on-site. However, if the primary costs (losses) are largely off-site, it will generally be cheaper to treat the effects of erosion than to prevent erosion on-site. The primary reason for this generalization is the "time lag" between when an on-site measure is implemented and when its effects are evident downstream.

Comment: (E. Casman, Interstate Commission on the Potomac River, Baltimore, Maryland) One of the reasons the above generalization made by Dr. Crosson holds is that benefit-cost analysis puts heavy weight on benefits today versus tomorrow. The government needs to take a longer-run view because it should represent future unborn generations.

Response: (P. Crosson) This is true, especially when the costs of erosion cannot be extracted from beneficiaries in an effort to compensate those who are harmed. However, it is also possible that additional information on the costs and benefits (measures of efficiency) would help reduce these equity issues.

Question: (J. Andersen, Utah State University, Logan, Utah) How are the issues raised above to be handled when the lands in question are "publicly owned", as is true in most of the Western United States?

Response: (P. Crosson) The key issue that has to be resolved when public lands are involved is the purpose for public ownership of these lands. There is potential for government to put undue weight on present uses. The government must consider all benefits and costs in both the long and short term. The key problem is determining what pattern(s) of use yields the greatest social dividend.

Technical Sessions



PREDICTIVE APPROACHES FOR LEACHING IN THE UNSATURATED ZONE

R.J. Wagenet¹, M.J. Shaffer², R.E. Green³

ABSTRACT

Historical and contemporary modeling approaches to estimation of solute leaching in unsaturated soils range from simple empirical methods to complex deterministic models that evolve from consideration of mass balance. The basic equations used in each generic approach provide insight into the major assumptions inherent in the models that result. The strengths and weaknesses of each modeling approach influence their use for research, action-agency, or management purposes. Future needs for improved leaching models useful for these purposes vary according to the user, but include better representation of tillage and other cultivation practices, improved estimation of key characterizing relationships of soil hydraulic properties, better representation of macropore flow and enhanced user-friendliness in models intended for use by non-scientists.

INTRODUCTION

Concern about groundwater contamination has focused attention on the processes that influence chemical fate in soil-water systems. Independent of the mode of introduction of the chemicals, a major concern with respect to groundwater contamination is the passage of these chemicals through the relatively thin layers of soil that cover many terrestrial surfaces. This water-unsaturated zone of the soil profile, extending from the soil-atmosphere interface to the water table, and including the normal root zone of most plants, is a chemically and biologically very active region of the biosphere. The residence time of chemicals within this region, and the processes operative within it, ultimately determine the degree of groundwater contamination. It is now recognized that only through a better understanding of the basic physical, chemical and biological processes of the unsaturated zone can we hope to better manage that portion of the system over which we have control, thereby minimizing groundwater contamination and associated risks to the public.

One fairly recent approach to summarizing and integrating the various processes operating in unsaturated soils has been to utilize simulation modeling techniques. When applied to the unsaturated zone, this has often given rise to a general class of models that can be termed leaching models. Such models in contemporary form usually begin with consideration of water infiltration and redistribution and the effects of plants upon water flow through extraction. The models then estimate solute (dissolved chemical) transport resulting from the calculated water fluxes, and include processes such as ion exchange, sorption, biological or chemical degradation, volatilization, chemical precipitation/dissolution and plant uptake. These models in their various forms serve as useful tools for the testing of hypotheses regarding basic relationships between the processes, demonstration of the interaction and interdependency of the processes for educational purposes, and assessment of chemical fate in the environment for regulators or decision-makers. The leaching models are all different, reflecting the bias and experience of the model developer, but are based upon the same relatively few basic principles. Review of these models will provide an appreciation of the evolution of existing approaches, and will allow an evaluation of the current state-of-art in the quest to predict the movement of chemicals to groundwater.

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HISTORICAL PERSPECTIVES

Leaching models have evolved from two general approaches: those models that are empirical, and those that begin from some consideration of mass balance.

Empirical Relationships

The reclamation of salt-affected soil in the semiarid western United States focused attention in the early 1950's upon the leaching of soluble salts. Data from field studies in the Coachella Valley of California (Reeves et al. 1955, Reeves 1957) suggested that salt leaching from soil followed a general pattern. The empirical equation derived to describe water required as a function of desired change in salt content was:

$$D_w/D_s = [0.20(EC_e)_0/(EC_e)] + 0.15 \quad [1]$$

where D_w = depth of water (L) leached through a depth of soil D_s (L),
 $(EC_e)_0$ = average saturation extract electrical conductivity (ds/m) of the soil depth D_s before leaching, and
 EC_e = average saturation extract electrical conductivity (ds/m) of the soil after leaching.

Subsequent studies modified this equation somewhat, and introduced the concept of an equilibrium EC that was the value of the electrical conductivity of the upper 5-10 cm of the soil profile after leaching had stopped. Its value was felt to depend upon the salinity of the irrigation water, evaporation and drainage. These equations showed some utility in field reclamation studies in several semiarid areas, and represented a first attempt at integrating irrigation, evaporation and the leaching of soil salts.

Studies of salinity have not been the sole source of empirical leaching models. Burns (1975), utilizing the concept of sequential uniform mixing, proposed a relationship showing the fraction (f) of surface-applied nitrate that will leach below a depth (h) in a textually uniform soil initially at field capacity water content (θ_{fc}) to be

$$f = [I/(I + \theta_{fc})]^h \quad [2]$$

where I = cumulative quantity of water (L) that infiltrated the soil.

This equation gave satisfactory agreement with data collected from the literature, can be used on most portable calculators and has been incorporated in a simple nitrogen calculator for growers. Burns has demonstrated the potential of this approach by showing how the variability in yield response data can be reduced by plotting yield against the amount of applied N calculated to remain in the profile after rainfall (using eq. 2) rather than simply against the rates of applied N Burns (1980).

Equations 1-2 provide only a very general approximation of leaching processes. These equations are restricted by factors which limit all empirical approaches, and are as a result rather non-quantitative with respect to masses of chemicals leached. However, they were (and are) particularly useful in cases where only a few measurements could be made, when only approximate estimates are needed, and when no other estimation tool is available. Where better estimates are required, these approaches have generally been superseded by the mass balance models reviewed below.

Models Based on Conservation of Mass

Leaching models based upon mass balance considerations evolved simultaneously from two different directions, although the philosophies of the two were quite similar. One path had its roots in salinity/reclamation issues, and represented an attempt to summarize leaching processes more universally than was done in equation 1. The other path originated in the column chromatography literature, and provided the basis for development of equations that describe simultaneous physical and chemical processes influencing solute displacement.

The general salt balance equation for downward salt movement in situations where no sources or sinks of salt exist:

$$\left[\begin{array}{c} \text{Change in mass} \\ \text{of salt in soil} \end{array} \right] = \left[\begin{array}{c} \text{Mass of salt in} \\ \text{added water} \end{array} \right] - \left[\begin{array}{c} \text{Mass of salt in} \\ \text{drainage water} \end{array} \right] \quad [3]$$

This can be expressed for a uniform soil profile as

$$D_s \Delta \theta (\Delta C_{sw}) = (C_{iw} D_{iw}) - (C_{dw} D_{dw}) \quad [4]$$

where D_s = depth of soil (L),
 $\Delta \theta$ = change in profile volumetric water content (L^3/L^3),
 ΔC_{sw} = change in salt concentration in the soil solution (M/L^3),
 C_{iw} = salt concentration (M/L^3)
 D_{iw} = depth of added irrigation water (L),

and C_{dw} and D_{dw} are similar with respect to the drainage water.

For non-uniform soils, equation 5 can be written as:

$$\sum_i D^i (\theta_{fc}^i C_{fc}^i - \theta_0^i C_0^i) = C_{iw} D_{iw} - C_{dw} [D_{iw} - \sum_i D^i (\theta_{fc}^i - \theta_0^i)] \quad [5]$$

where i = a superscript that refers to the i th soil layer,
 D^i = thickness of a soil layer (L),
 fc = a subscript that refers to field capacity water contents and salt concentrations, and
 0 = a subscript that refers to the initial water content and salt concentration.

Equations 4 and 5 served as the basis for early leaching models. With several assumptions about the nature of the leaching process, equations were derived which described reasonably well the release of readily soluble salts (evaporites) from a saline soil during leaching. These approaches accounted for approximately 80-90% of the total salt in the profile, but were limited in their ability to describe the concentration of salt in drainage waters.

The concentration of the drainage water C_{dw} is often of critical interest to nonpoint-source pollution of groundwater. Van Der Molen (1956) used equation 5 as the basis of a simple model of water and salt movement. He assumed that all added irrigation water mixed completely with the resident solution of the first soil layer. The resultant solution in excess of field capacity moved into the second layer as drainage water, and mixed with the solution initially present in the second layer. Repetition of this process for i soil layers provided C_{dw} at the lower limit of consideration. By contrast, Terkelstou and Babcock (1971) assumed that upon application, only that amount of irrigation/drainage water was added to the first/next layer which brought the layer to field capacity. This process continued until the lowest layer achieved θ_{fc} . Alternative approaches were even simpler; Bresler (1967) calculated C_{dw} as

$$C_{dw} = (C_0^i + C_{fc}^i) / 2 \quad [6]$$

and Bresler and Hanks (1969) as

$$C_{dw}^i = (C_0^i \theta_0^i + C_{fc}^i \theta_{fc}^i) / (\theta_0^i + \theta_{fc}^i). \quad [7]$$

These simplified layer-type models provided straightforward methods to estimate salt distributions in soil during leaching. They suffered somewhat from the lack of consideration of mediating processes (such as precipitation/dissolution or ion exchange). However, these limitations did not preclude their use, as most early salinity studies were accomplished in soil systems at or near-equilibrium between solution and exchangeable or precipitated phases. An additional weakness of these approaches was that time was not included as a variable in the equations. Leaching in these models was event-driven, not a continuous process (as in nature) of infiltration and redistribution of water and solutes. Additionally, these early models included a built-in dispersion process, as the selection of depth intervals used in assigning the i layers influenced the calculated transport of salt. This problem still remains today with some leaching models, now takes the form of numerical dispersion resulting from inaccuracies in finite difference solutions. Even so, the early leaching models were useful tools in assessing the general movement of inorganic salts in relatively saline soils. This approach, as will be seen below, was insufficient for description of leaching in systems characterized by highly transient fluxes of water and solute.

The parallel path of development of leaching models based upon conservation of mass originated in the field of column chromatography. Chromatographic models can generally be classified as either plate theories or rate theories, with an excellent review of the distinctions being given by Frissel and Poelstra (1967).

Plate models consider a chromatographic (or soil) column as being divided into a large number of plates. Two phases are presumed in each plate, sorbed and liquid, with equilibrium between the two. It is immaterial whether an exchange process, diffusion process, or any other process is considered as the main dispersion process during flow through the column. This assumption means that there is only one unit length (plate height) to which this definition applies. If the height is too long, the concentration is not uniform, if too short no equilibrium exists between the two concentrations.

Chromatography models based upon the plate approach have been developed by Martin and Synge (1941), Mayer and Tompkins (1947) and others. The models, quite useful in chromatography applications, presume that flow occurs through adjacent and consecutive plates, with equilibrium in each plate achieved before flow passes to the next plate. This approach, analogous to the simple layer-type models used in early salinity studies, suffers the same weaknesses with respect to simulation of soil leaching processes. That is, the simplification of transport (leaching) to the point of a "discontinuous" plate flow can lead to serious cumulative errors as calculation proceeds to long depths (numerous plates) or times. This has generally prevented much of the early chromatographic literature based on plate theories from being directly applicable to a wide variety of soil leaching processes. A notable attempt by Dutt and Tanji (1962) to describe salt leaching was based upon plate theory. Additionally, several investigators (Rible and Davis 1955, Bower et al. 1957, Thomas and Coleman 1959) applied these models to the description of ion distribution between exchange and solution phases during flow. These studies failed to consider the mixing that takes place as a result of pore water velocity distributions (resulting from pore size and shape variations). Additionally, in all of the above cases displacement and ion exchange under partially water-saturated conditions, which normally prevail in soil, were not considered. Even so, fairly good agreement between measurement and theory was obtained for the few cases considered.

The evolution of the "discontinuous plate theory" into the "continuous plate theory" was presented by Glueckauf (1955) in the form:

$$\frac{\partial c}{\partial x} + a \frac{\partial c}{\partial V} - \frac{\Delta x}{2} \frac{\partial^2 c}{\partial x^2} = 0 \quad [8]$$

where a = distribution coefficient between sorbed and solution phases,
 V = volume of solution added to the column, and
 Δx = volume of a theoretical plate.

Glueckauf's analytical solutions to equation 8 provided continuous description of $C(x,t)$. The work of Van Der Molen (1956) built upon equation 5 using the continuous plate concept as a basis for a leaching model of the reclamation process in Dutch polders. This applications of Glueckauf's method was possible due to the unique initial (saturated soils) and boundary condition (pounded water) of Van Der Molen's case. Gardner and Brooks (1957) modified the Glueckauf theory and considered the soil to be composed of both mobile and relatively immobile phases. They concluded that soil leaching processes are dominated by dispersion at the flow velocities that normally occur during leaching, an observation consistent with the development of contemporary leaching models that include a dispersion-diffusion component.

The advantage of the plate theory is also its limitation. That is, while the plate height can be easily determined experimentally, the approach does not lend much insight into basic processes, nor does it allow one to predict the effects of changing one or more of the controlling soil water variables, such as pore-water flow velocity. By contrast, in the rate theories a physical model of the system is required, with each parameter in the model either known beforehand or measured in the experiment. This has led to development of contemporary leaching models primarily from rate theories, with the most important early contributions made by DeVault (1943), Heister and Vermeulen (1952), and Lapidus and Amundson (1952). These models form the basis of the diffusion theory now used in many contemporary leaching models. Comprehensive reviews of the development of such theories exist elsewhere (van Genuchten and Cleary 1979, Nielsen et al. 1986).

CONTEMPORARY APPROACHES

Water Movement

The beginning objective of contemporary models of solute leaching in field soils, to which the balance of this discussion will be limited, is an accurate estimation of water movement. This initial step, properly accomplished, provides calculated water fluxes and water contents that can be used to estimate the simultaneous leaching of solutes dissolved in the water. A variety of leaching models evolve from the different approaches that can be taken to estimating water movement. Before considering specifically the estimation of chemical movement, the limitations in our ability to estimate water movement should be recognized.

One commonly-used approach to estimating water movement utilizes the one-dimensional equation for transient vertical water flow, derived from Darcy's Law and the equation of continuity as:

$$\partial \theta / \partial t = \partial / \partial x [K(\theta) \partial H / \partial x] \quad [9]$$

where H = total hydraulic potential (L), composed in this case of the sum of matric (h) and gravitational (g) potentials;
 $K(\theta)$ = water content-dependent hydraulic conductivity (L/T); and other terms have been defined.

This equation can be solved numerically to give $h(x,t)$ as a function of the soil initial and boundary conditions, and soil water properties. Estimation of $h(x,t)$ automatically gives $\theta(x,t)$, provided the soil water characteristic curve $[\theta(h)]$ is known. Knowledge of $\theta(x,t)$ allows the soil water flux q (L/T) to be calculated.

Use of equation 9 to estimate $\theta(x,t)$ and to eventually calculate $q(x,t)$ depends upon accurate knowledge of both the $K(\theta)$ relationship and the gradients $(\partial H/\partial x)$ that exist under field conditions. Without dependable information on these, the use of equation 9 to estimate field-scale fluxes must be carefully considered. Recent work by many soil scientists, beginning with Nielsen et al. (1973), has shown that $K(\theta)$ can be variable by orders of magnitude over the space of a single field. Similarly, gradients are spatially variable at any one time. This has led to the realization that calculated field-scale estimates of $\theta(x,t)$ and $q(x,t)$ may be quite tenuous in many cases. It is unresolved how important these inaccuracies are in the estimation of chemical leaching to groundwater over broad areas. It appears that in some cases the error in predicted mass fluxes may be large, while in others the impact may be less important. We will return to this point below.

As an alternative to use of equation 9, simpler methods have been proposed to calculate water movement in soil. As will be discussed below, these approaches are utilized when only approximate estimation of water movement is required. These models generally consider a simple water balance, and are analogous to the water flow conceptualizations used in early salt leaching models. Added water moves into a designated soil layer until a certain water content (e.g., field capacity or saturation) is achieved, with any excess water free to move into the next layer. These models are usually episodic in nature, with the driving force for water flow (and eventually solute leaching) being the addition of water to the system. The attractiveness of these methods are that they eliminate the need for knowledge of the $K(\theta)$ relationship and hydraulic gradients. Perhaps just as important to those who utilize this approach, it greatly simplifies the numerical algorithms necessary to calculate water flow. This also allows other hydrologic processes, such as runoff and snowmelt, to be included in the model with much more ease than they can be added to more mechanistic models.

Both approaches offer strengths and weaknesses. The gradient/flux models developed from Darcy's Law are generally quite computer-intensive, have more demanding input data requirements (e.g. $K(\theta)$ and $\theta(h)$ relationships), and are often difficult to transfer between users (although this is less of a problem than it used to be). On the positive side, they provide the opportunity to clearly test the sensitivity of calculated $q(x,t)$ and $\theta(x,t)$ to different $K(\theta)$ relationships, and to represent the influence (e.g., through multiple executions) of spatially variable hydraulic properties. The water balance approaches demand less data, and are easier to execute and transfer between computers. The simplification of the basic process included in these models certainly changes estimated $q(x,t)$ and $\theta(x,t)$ from what would be obtained with the Darcy flow-based models.

It is important to recognize that, with few exceptions, the great bulk of water flow modeling efforts have focused on homogeneous soils. However, within the last ten years field observation of water flow has convincingly demonstrated that not all soils behave according to the "classical" concept of water flow. In fact, for well-aggregated soils, it is clear that a relatively few large openings (macropores), arising from a variety of sources, can result (depending on the boundary conditions) in water and chemical movement at a rate far exceeding estimations based upon the gradient/flux calculations used for flow in homogeneous soils. At the same time, it has been observed that there can be, under certain conditions, substantial water movement through such soils without displacement of resident chemicals. Quantitative approaches to describe the movement of water and leaching of chemicals in these systems are currently limited, with only a few published treatments of the mechanics of water movement (Edwards et al. 1979, Beven and Germann 1981, White 1985). Improved models of these systems are needed, as it is becoming apparent that at least a part of the observed spatial variability of water flow that precludes use of "classical" models

based upon equation 9 is in fact due to macropore transport processes. It is interesting to note that although there are a number of software packages available for estimating water movement in homogeneous soil and layered soils, there are not any known to these authors that are widely recognized as useful tools for macropore systems. Recent approaches by van Genuchten (1985) and van Genuchten and Dalton (1986) offer promise in this area.

Solute Leaching

As with water flow, there is a classical and widely-used beginning point for solute leaching models. There are also simplified approaches that are generally used for nonquantitative purposes.

A wide variety of mechanisms must be considered in predicting solute leaching. The most often used of the several theoretical approaches that have been developed is miscible displacement theory. This representation of solute displacement as the combined processes of chemical diffusion and mass flow can be traced to chromatography through the rate-theory studies cited above. In the early 1960's the theory was extended to questions of solute displacement in soils and was found reasonable in several soil types under a range of laboratory conditions. The approach was later expanded to include nonsteady flows of water and solute and to descriptions of sources or sinks of solute that act during transport. The usefulness of the basic approach, particularly for carefully controlled laboratory situations of solute transport, has been reinforced by a large number of subsequent investigations (summarized by van Genuchten & Cleary 1979, Nielsen et al. 1981). The equations arising from this work and used as a basis of many leaching models are interchangeably known as miscible displacement, dispersion-convection, or solute transport equations.

Miscible displacement theory assumes that a solute being transported through soil is subject to two types of mixing processes within the pores. One is chemical in nature, resulting from the diffusion of solute in response to concentration gradients existing in soil solution. The other is physical in nature resulting from variations in water flow velocity within each pore and between pores. These two mixing processes occur simultaneously during the imposed mass flow of solute in response to the movement of the bulk soil water. With these fundamental assumptions, a wide variety of solute leaching models developed from miscible displacement theory have been reported (reviews by Nielsen et al. 1981, Addiscott and Wagenet 1985, Wagenet and Rao 1988). Depending upon the model, water flow can be described as both a redistribution or evaporative process, and solutes can interact with the soil surface (via adsorption or ion exchange processes), be transformed by chemical or biological reactions, precipitate or dissolve (generally limited to inorganic ions), volatilize, or be taken up by plants. In general terms, these processes can then be rewritten (in the example of a pesticide) as:

$$\frac{\partial}{\partial t} [\rho s + \theta c + \epsilon c_g] = \frac{\partial}{\partial x} [\theta D(\theta, q) \frac{\partial c}{\partial x} - qc - D_g(\epsilon) \frac{\partial c_g}{\partial x}] + \phi \quad [10]$$

where s = sorbed phase concentration (M/M),
 c_g = gas phase concentration (M/L³),
 $D(\theta, q)$ = combined dispersion-diffusion coefficient for solute in the liquid phase (L²/T),
 D_g = diffusion coefficient in the gas phase (L²/T),
 ϕ = represents a source (+) or sink (-) of pesticide (T⁻¹),
 ρ = soil bulk density (M/L³), and
 ϵ = gas-filled porosity (L³/L³).

The use of equation 10 as the basis for a solute leaching model suffers from limitations similar to those of concern with water flow models built upon equation 9. That is, the relationship between water flux, water content, and the apparent diffusion coefficient is subject to the same spatial

variability as the $K(\theta)$ relationship. Field studies of $D(\theta, q)$ (Biggar and Nielsen 1976) illustrate that a population of values measured at the maximum water content and water flux achievable by ponding is in fact a skewed distribution. The resultant vertical distribution of chemical in the soil profile therefore varies within each one-dimensional leaching region of a field in which leaching occurs. Additionally, leaching models constructed from numerical solutions to equations 9 and 10 not only require information on the $K(\theta)$ and $\theta(h)$ relationships, but also on the nature of the $D(\theta, q)$ relationship. The situation then exists that at any x-y-z coordinate location in a field, the values of θ and q are uncertain and dependent upon pore geometry considerations that prevent any single K - θ - h or D - θ - q relationship from necessarily being correct. Given the uncertainty that exists in the "true" field-value of these relationships at any spatial location, it has become clear that any attempt to predict with certainty the solute flux at a particular field spot will be a tenuous, if not impossible, exercise. A more reachable goal would be to predict mean values for solute flux and concentration over an entire field or research plot. The uncertainty associated with these values would be reported as an aid in interpretation and as a guide in management decisions. This is an obvious area for both current and future research emphasis, with substantial effort currently focused on estimating K - θ - h over large areas, development of models that consider the uncertainty in K - θ - h relationships, and identification of alternative approaches to description of leaching.

Most alternative approaches that have been developed are consistent with the water balance alternative to Darcy's Law. One method is simply

$$q_s = q (C_i + C_{i+1}) / 2 \quad [11]$$

where q_s = solute flux ($M/L^2 \cdot T$)
 C_i and C_{i+1} = solute concentrations (M/L^3) at adjacent positions i and $i+1$ in the soil, and
 q = determined from water balance calculations.

This approach is used only for very approximate purposes in cases where very little field information is available. More often, the episodic nature of solute movement in these alternative approaches is better represented through the use of a piston flow approach. In this type of model, the spreading of the solute pulse resulting from hydrodynamic dispersion can be either ignored or not, depending upon the purpose of the model. If the purpose is only to estimate the position of the solute pulse (either the peak or the leading front), then for a solute that sorbs to the soil (Wagenet and Rao 1988):

$$x_i = x_{i-1} + [(I_i - I_d) / \theta_{fc} R_F]; \quad I_d < I_i \quad [12]$$

$$x_i = x_{i-1} \quad I_d \geq I_i \quad [13]$$

$$I_d = \int_0^{x_i} [\theta_{fc} - \theta(x)] dz \quad [14]$$

where x_i and x_{i-1} = the depths at which the solute pulse is located after the i -th and $(i-1)$ -th events;

I_i = amount of water (L) infiltrating into the soil profile for the i -th event;

I_d = amount of soil-water deficit (L) resulting from plant extraction of water above depth x_i ;

$\theta(x)$ = volumetric water content distribution within the root zone; and

R_F = retardation factor to account for sorption effects.

Equations 12-14 can be expanded further into approximate solute leaching models that estimate concentrations. DeSmedt and Wierenga (1978) have presented some approximate methods that

can be used to include description of solute dispersion during transport, and these can be employed to estimate solute concentration once the value of x_i has been identified. In general, these concepts hold in soils without macropore transport of water and solutes. They are very useful approaches for approximate purposes, such as demonstrating that water leaving a field as leachate during a water application event does not generally contain solute present at the soil surface prior to the water application. The leachate is, rather, that water already present in the soil profile prior to the water application. These models are presently limited to non-quantitative uses, although their usefulness would be enhanced by deriving them with consideration for the field-measured uncertainty in their component processes. For example, water flux or retardation factors could be represented as expected mean values, with associated variance. The resulting model would then calculate concentrations in terms of an expected mean and variances. This approach remains to be developed and tested.

EXISTING MODELS

Classification of existing models can be approached from several perspectives. The preceding discussion reviewed the evolution of solute leaching models, and contrasted the level of rigor used to represent key processes. From a modeler's perspective, this is a logical approach to classification, as the level of rigor often reflects the degree of understanding of basic process. The bias and training of individual modelers becomes apparent in such cases. In the past, it was sufficient to classify models on such a basis, as developers of the models were in almost all cases also the (only?) users of the models.

This situation has changed dramatically with the development of affordable, usable mini- and microcomputers. A wide range of professionals inside and outside academia are now interested in and capable of using models developed elsewhere. These users have different needs, and models of solute leaching have been adapted or derived and then employed in response to these needs. The number of such models has increased dramatically over the last few years, yet the level of rigor utilized is often similar according to the expected use of the model. As a result, it appears that contemporary solute leaching models can be logically grouped into three classes based upon users: researchers, action agencies and a general class of extension/farm users.

Research Models

The development of solute leaching models applicable to field conditions became a focus of both academic and federal research efforts in the early 1960's. Dutt (1961) was an early pioneer in combining a relatively complex chemical equilibrium source-sink approach with plate theory to predict salt transport in soil columns. This work combined with the basic work on miscible displacement reported by Nielsen and Biggar (1961), generated increased interest in analytical and numerical solutions to Richards' equation and resulted in the development of additional models for water and solute transport (e.g., Hanks and Bowers 1962, Nielsen and Biggar 1963, Bresler 1967). Among these, the simulation model for biophysicochemical processes in soils reported by Dutt et al. (1972) and extended by Shaffer et al. (1977) to include aquifer systems, was not only a precursor for other multiple-process simulation models, it was also widely used during the 1970's to conduct environmental impact studies on the quantity and quality of return flows from proposed irrigation projects.

In the early to middle 1980's, the Nitrogen-Tillage-Residue Management (NTRM) model (Shaffer et al. 1983, Shaffer 1985, Shaffer and Larson 1987, Swan et al. 1987) was developed as an extension of the previous irrigation return flow model IRFSM (Shaffer et al. 1977, Shaffer and Gupta, 1981). Among other processes, NTRM includes crop growth and leaching of $\text{NO}_3\text{-N}$ and major cations and anions. GOSSYM (Baker et al. 1985, McKinion and Baker 1983) simulates cotton growth and contains a two-dimensional Darcy's Law submodel for water movement with

convective transport of nitrates and implicit dispersive nitrate transport. Other, similarly comprehensive models such as CREAMS (Knisel 1980), GLEAMS (Leonard et al. 1986), EPIC (Williams et al. 1983) and PRZM (Carsel et al. 1985) have also been developed to include solute leaching in a broader assessment of natural processes, but are generally considered to be action-agency models, rather than models useful to the research community in extending understanding of basic processes.

There has been an explosion of leaching models in the research community since the mid-1970's. One example of such models is LEACHM (Wagenet and Hutson 1987), which has been formulated to provide the opportunity to describe the leaching of nitrogen fertilizers, pesticides, or inorganic salts, depending upon the interests of the users. This model is somewhat unusual as a research model, as it has been designed for use by persons other than the developers. Other research models are often a component of larger soil-plant simulation modeling efforts. These research models, which include description of solute transport, are generally complex, integrated process models requiring relatively high levels of professional expertise for their operation and interpretation. Users of these models tend to be the developers, the scientists they have trained, or other scientists in the same or related disciplines. The solute most commonly modeled appears to be $\text{NO}_3\text{-N}$. However, this situation is changing as more emphasis is currently being placed on organic chemicals. Depending on the type of study being conducted, one or more of these models could be selected as being the most appropriate.

Research models that focus on solute leaching usually include appropriate formulation of equations 9 and 10. These models include plant growth in response to transient water regimes, nitrogen movement and transformation, management of irrigation water and salts, disposal of wastewater, and pesticide leaching and transformation. Equation 10 has also been adapted to describe solute transport in soils with mobile and immobile water phases (van Genuchten and Wierenga 1976) though the results have been validated only against laboratory column data. Fast preferential water flow in the macropores of field soils was treated by Beven and Germann (1981) using an equation similar to equation 9 in the context of domain theory. As mentioned above, their approach has not yet been extended from water to solute flow.

The integrated process models tend to be quite similar from a general standpoint. Most of these models include some type of numerical solution to the basic partial differential equations for water and solute transport. Convective transport is simulated, with implicit or explicit description of dispersion, and source-sink terms for chemical, biological, and physical removals and additions of water and solutes. FORTRAN seems to be the common computer language used for these models. However, various versions of FORTRAN are known to exist, and the number and types of subroutines used varies widely. In addition, some models tend to be unbalanced (overly complex) in detail for a particular component of the system, depending upon the discipline of the primary developer.

Action-Agency Models

These models generally incorporate simplified algorithms for processes included in the research models, and in a few cases may address areas not yet covered by the research simulators. These models are used by action agencies to assist with planning and regulatory functions. In general, the same processes included in the research models are covered in these models. The water flow solution technique tends to be either storage routing or piston flow with implicit dispersion, and either pesticides, $\text{NO}_3\text{-N}$, or major inorganic ions are the solutes of interest. The interfaces with the user tend to be more highly developed than with the research models, and the action agency models tend to execute more rapidly for each year simulated. The interface between the user and the model is very important because routine use of the model cannot tolerate an inefficient interaction between the model and user. Some specific examples of these models include the

IRFSM model used by U.S. Bureau of Reclamation, the CREAMS, GLEAMS, EPIC and SWAM (Alonso and DeCoursey 1985) models used by SCS, and PRZM used by the USEPA.

Of particular interest to the regulatory process with respect to pesticide leaching has been the Behavior Assessment Model (BAM) of Jury et al. (1983). This is essentially an analytic solution of equation 10 formulated to include the relevant pesticide fate processes of sorption, degradation, and volatilization. This "model" can be used only to categorize the relative behavior of pesticide under the specific conditions and assumptions used in developing the analytic solution. The attraction of such a model lies in the relatively few data required to characterize pesticide behavior, and the relative ease of programming an analytic solution. When correctly used, a screening model can provide the opportunity to segregate pesticides into behavioral classes, within which their behavior in the field may be inferred from similarly classed, but better studied pesticides. However, such models have been incorrectly used to estimate environmental fate under field conditions, a use for which they were never intended.

Extension/Farm/User Models

There is substantial interest in using models to guide the application of water (both saline and non-saline) and pesticides to soils and crops, and to predict the fate of these materials in the environment. The wide availability of microcomputers and increased recognition (through educational programs) of the complexity of soil-plant-water systems has accelerated the demand for accurate, yet usable, management models of these systems. Research over the last fifteen years has provided some insight into the processes operating under field conditions. Several attempts have been made to condense this information and utilize it for broader agricultural and environmental purposes.

Extension/Farm/User models are intended to provide site-specific management assistance to farmers, the lay public, or persons advising these groups. As such, solute leaching is represented in very simplistic terms. These models generally use a water balance or piston flow approach, and the emphasis is not on quantitative predictions, but on providing the opportunity to compare alternative practices or situations. Given these constraints, use of these models for regulatory purposes is undesirable. The interface with the user is of extreme importance, and the model must be relatively easy to understand and use. Model algorithms are generally flexible and allow modification by extension personnel and others at the local level.

An excellent example of a model intended for on-farm management that includes the effect of management alternatives upon solute leaching is the COFARM (Coordinated Farm and Research Management) model (Shaffer et al. 1984). COFARM provides farm management assistance in the areas of nitrogen fertilizers, nitrate leaching, tillage, crop residues, crop yields, and soil erosion for systems cropped with corn. Other models in this category are MOUSE (Steenhuis and Pacenka 1987) and the microcomputer-based management model for chemical movement, CMLS, developed by Nofziger and Hornsby (1986).

FUTURE RESEARCH NEEDS

Estimation of solute leaching in soil is clearly evolving from an experimental science into a computational exercise. Only a limited number of field measurements are available that can be used to confirm or deny any solute leaching model, and there is substantial question whether the validation of a model in a limited number of field cases will assure the ability to predict correctly in most cases. There will probably continue to be a dearth of field data of solute concentrations in both the vadose and saturated zones. Individuals interested in estimating solute leaching, whether for research, regulatory or user purposes, will therefore be forced to rely more heavily

upon computational methods, with occasional access to a limited set of data that will either encourage or discourage use of a given model.

Given this reality, it seems prudent to carefully examine future needs by user groups. It seems clear that model development will continue to be largely an exercise of the academic and federal research community, with the results of research model-building filtering to user groups. The filtering process should eventually provide modeling approaches with increased utility and in which we can have (it is hoped) increased confidence of accuracy.

Research Models-Future Areas of Focus

The greatest challenge in modeling leaching will continue to be accurate prediction of water fluxes and water contents in the unsaturated zone. It appears that these fluxes are more often spatially variable when leaching fractions are high, or when plants are not extracting substantial amounts of water (Dudley et al. 1981). That is, the lower the flux, the less variable it is, and the more appropriate is the representation of water flow as a deterministic, one-dimensional, mechanistic process. In such cases, Eqs. 9 and 10 may well be reasonable approaches. Yet, it is clear that $K-\theta-h$ relationships can be quite variable, and this will translate into variable water fluxes, and similarly variable solute fluxes, under some conditions. Leaching models need to be developed to describe each type of situation, and the critical issue is the manner in which soil-water flow is represented.

Accurate estimation of solute leaching depends to a great degree upon the processes active within the first 30 cm of the root zone. This shallow zone is not well modeled in most solute leaching models, particularly with respect to the effects that tillage and other cultural practices have upon it. Given the importance of this region, research simulation models of solute leaching in the unsaturated zone should be extended to routinely include two dimensions, consideration of shallow water tables, and incorporation of a complex geometry for the upper soil boundary. The finite element approach seems to be promising, due to its capabilities with complex boundary geometry. Models need to be able to simulate the upper boundaries associated with ridge-till, irrigation, and other tillage and cultural practices. The two-dimensional case is also needed to more fully account for surface runoff-runon relationships, lateral flow along subsurface layers, and the complex upper boundary. Additionally, a simultaneous unsaturated zone and aquifer simulation is needed to properly account for sub-irrigation and the exchange of solutes between surface and groundwater.

Alternative formulation of research models must be considered for representation of the spatial and temporal variation in soil and water flow processes. Stochastic models of the type of Jury (1982) and Jury et al. (1982) or Knighton and Wagenet (1987a,b) need to be tested on a wider basis as possible tools useful in estimating solute leaching. The models should include stochastic input generators for model-driving variables and model coefficients. The assumption should no longer be made that mean or other central values for model inputs and coefficients will produce representative output from non-linear simulation models. The development of these models will only be possible within the context of the interpretation of further field experiments aimed at quantification of spatial and temporal variability of solute leaching. Stochastic inputs will be useful in testing either mechanistic models used in an "ad-hoc" stochastic manner (e.g. through Monte-Carlo techniques) or stochastic models.

Considerably more field and laboratory research is needed to quantify the biological and chemical processes associated with pesticide degradation and sorption in natural field systems. Additionally, the relative importance of exchange and precipitation/dissolution reactions in mediating spatially variable fluxes of dissolved solutes needs to be better understood to place water flow variability and solute leaching variability in proper perspective. We need this information before existing and future leaching models can be properly evaluated.

Improved methods of measuring key relationships, such as the $K(\theta)$ relationship, are needed. In-situ techniques that can be used on multiple sites over a large area without excessive cost are essential if better estimates of water flux are to be obtained. Alternatively, improved methods of accurately inferring soil hydraulic properties from soil survey information would greatly aid in applying any new stochastic approaches to relatively unstudied sites.

The topic of macropore flow needs to be investigated more completely from the modeling perspective. We need more information on how to simulate the interactions between the biological, chemical, and physical processes operating in this type of system. For example, how should exchange of water and solutes between the macropores and soil peds be simulated? When should we be using different microbial population sizes and microbial access to nutrients, carbon dioxide, and oxygen? How does the presence of macropores affect the freezing and thawing of soils and associated leaching events? Is the assumption, so frequently used, of an instantaneous and reversible equilibrium between solution and sorbed phases valid?

Action Agency Models - Futures Areas of Focus

Regulators need both simple and complex models. Site-specific models, often more simple in their design, may need to be applied quickly and with little information to obtain "best guess" estimates of the response of a particular system. However, regulatory agencies often use models for generic-type analyses of, for example, classes of pesticides in different hydrologic settings. These models must, by their nature, be complex in order to incorporate all relevant process and provide an estimate of the influence of the natural (spatial and temporal) variability of the system. When these types of models are used for regulatory purposes, it is particularly important to consider the uncertainty in the input parameters and the knowledge of basic processes, and to associate an uncertainty with the model output.

One of the most important consequences of improved research models will be development of simplified versions of these models for use by action agencies. As these models become available, several additional issues also need to be addressed. Improved user-friendly interfaces with expert system technology incorporated into their structures are needed and should be developed in cooperation with the intended users. The users should be provided with quantitative measures of the uncertainties associated with the model results. One approach (which probably would be included in improved research models) would be to develop families of confidence intervals for a range of model input values routinely used in model applications. In all these developments, it will be extremely important that the limitations of a modeling approach be clearly established if action agencies are to make intelligent decisions based upon model results.

Extension/Farm/User Models - Futures Areas of Focus

Work is needed to develop algorithms and user interfaces suitable for computer applications at this level. The current practice of using the computer to display the contents of existing handbooks and fact sheets may not be an optimal method of technology transfer. In addition, a simple downsizing of research or action agency models may not produce a tool suitable for routine use at this level.

The development of expert systems technology offers the opportunity for incorporating research models of solute leaching into a package useful for routine management purposes. As such technology becomes more readily available, it may be possible to exploit the substantial experience with leaching models, while avoiding the current aspects of these models (large data demands, computer execution time) that limit their usefulness for routine purposes. Development of improved on-farm management of water and chemicals may result from progress in this area.

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SOLUTE TRANSPORT IN THE VADOSE ZONE: A REVIEW OF MODELS

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ABSTRACT

A number of conceptual models for solute transport in soil are reviewed, compared and categorized deterministic and stochastic, mechanistic and functional approaches. Thirty two models (characterized from an international survey) are analyzed in terms of their physical and chemical model components, their verification, and their applicability to field-scale problems. The models show great diversity in complexity and general applicability to field situations. Few models have been validated and few data sets are available for testing the models. Future research efforts directed toward validation studies of the models on a field scale (rather than developing still more complex models) are strongly encouraged.

INTRODUCTION

The importance of the unsaturated (vadose) zone as an inextricable part of the hydrologic cycle has long been recognized. Theoretical and experimental studies on both water flow and solute transport in this zone have been further motivated by attempts to manage the root zone of agricultural soils optimally as well as by concerns about soil and groundwater pollution. These studies have greatly increased our conceptual understanding of the many complex and interactive physical, chemical and microbiological processes operating in the unsaturated zone. They have also led to a large number of models which vary widely in their conceptual approach and degree of sophistication, and are strongly influenced by the environment, training and preoccupations of their developers.

The variety of approaches to modeling leaching was recently reviewed by Addiscott and Wagenet (1985). In their review a key distinction is made between deterministic models which assume that a system behaves in such a way that the occurrence of a given set of events leads to a uniquely-definable outcome, and stochastic models, which presuppose the outcome to be uncertain and are structured to account for this uncertainty.

A second main distinction is between mechanistic and functional models. Mechanistic implies that the model takes into account the most fundamental mechanisms of the processes, as presently known and understood (e.g. Darcy's law for water flow, combination of mass-flow and diffusion-dispersion mechanisms for solute transport). The term functional refers to models that incorporate simplified treatments of solute and water and make no claim to fundamentality. However, their use requires less input data and computer expertise as compared to mechanistic models.

Additionally, it may be useful to distinguish between models that are primarily research tools (most of the mechanistic models) developed either to aid the testing of assumptions or to contribute to better understanding of the physical processes, and those (functional models) that are mainly useful as guides to the management of soil and water resources.

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No attempt is made at an exhaustive literature review. The first part of our paper contains some basic descriptions of these various approaches. This is followed by a review of 32 models, resulting from a survey conducted through a questionnaire sent to 87 colleagues from 25 countries. Finally some challenging problems to be solved in the future are identified.

DETERMINISTIC AND MECHANISTIC MODELS

One-dimensional, vertical unsaturated-zone transfer processes are traditionally described at the macroscopic scale by the classical Darcian-based equation for water flow :

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left\{ K(h) \left[\frac{\partial h}{\partial z} - 1 \right] \right\} + A(z,t) \quad [1]$$

and the Fickian -based convection- dispersion equation for solute transport:

$$\underbrace{\frac{\partial(\rho S)}{\partial t}}_{(a)} + \underbrace{\frac{\partial(\theta C)}{\partial t}}_{(b)} = \frac{\partial}{\partial z} \left[\underbrace{\theta D_s}_{(c)} \frac{\partial C}{\partial z} \right] - \underbrace{\frac{\partial}{\partial z} (J_w C)}_{(d)} + \underbrace{\sum \phi_j}_{(e)} \quad [2]$$

Table 1 summarizes the main equations on which most of the deterministic and mechanistic models are based for both transient and steady-state water flow conditions as well as for interactive and inert solutes, subject or not to transformations.

In these equations:

h	=	water pressure head (positive in the saturated region, negative in the vadose zone) [L]
$C(h)$	=	capillary capacity; the slope of the soil water retention curve $\theta(h)$ [L^{-1}]
θ	=	volumetric water content [$L^3 L^{-3}$]
$K(h)$	=	soil hydraulic conductivity [$L T^{-1}$]
$D(\theta)$	=	capillary diffusivity [$L^2 T^{-1}$]
J_w	=	volumetric water flux density [$L T^{-1}$]
$A(z,t)$	=	water sources and sinks, notably those resulting from plant water extraction in the soil root system [T^{-1}]
z	=	vertical distance, positive downward [L]
t	=	time [T]
$C [ML^{-3}]$, $S [MM^{-1}]$	=	concentrations of solute associated with the solution and the solid phases of the soil respectively
ρ	=	soil bulk density [ML^{-3}]
J_s	=	solute flux density [$ML^{-2} T^{-1}$]
D_s	=	apparent dispersion coefficient [$L^2 T^{-1}$]
V	=	J_w/θ = the pore water velocity [$L T^{-1}$]
ϕ_j	=	rates of solute removal or supply [$ML^{-3} T^{-1}$]

In equation 2, terms (a) and (b) describe changes in sorbed and dissolved concentrations, respectively, (c) accounts for hydrodynamic dispersion, (d) is the advection of solute and (e) includes chemical reactions (such as precipitation/dissolution, and complexation).

Equations 1 and 2 are tentative in several aspects, some of which will be discussed throughout the paper. They form the general bases for modeling the transient, coupled water and isothermal-solute movements in the vadose zone.

The physical solute transport model (eq. 2) is coupled with chemical submodels through terms (a) and (e), briefly reviewed below.

Table 1.
Basic equations of the deterministic and mechanistic models.

<u>Flux equations</u>			
	<u>Water (J_W)</u>		<u>Solute (J_S)</u>
$J_W = \text{or}$	$-K(h) \left[\frac{\partial h}{\partial z} - 1 \right]$	[1a]	
	$-D(\theta) \frac{\partial \theta}{\partial z} + K(\theta)$	[1b]	
			$J_S = -D_S \theta \frac{\partial C}{\partial z} + J_W C$
			[II]
<u>Transient Transport Equations</u>			
Richards:			
	$C(h) \frac{\partial h}{\partial t} = - \frac{\partial J_W}{\partial z} + A(z,t)$	[IIIa]	$\frac{\partial T}{\partial t} = - \frac{\partial J_S}{\partial z} + \Sigma \phi_j$
			[IVa]
or			$T = \rho S + \theta C$
			[IVb]
Fokker-Planck:			S and C are linked through submodels <u>inert solute; no transformation.</u>
	$\frac{\partial \theta}{\partial t} = - \frac{\partial J_W}{\partial z} + A(z,t)$	[IIIb]	$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial z} \left(\theta D_S \frac{\partial C}{\partial z} \right) - \frac{\partial}{\partial z} (J_W C)$
			[V]
<u>Steady Water Flow Conditions</u>			
$J_W = \text{Const.}; \theta = \text{Const.}$			$- \frac{\rho}{\theta} \frac{\partial S}{\partial t} + \frac{\partial C}{\partial t} = D_S \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial z} + \frac{1}{\theta} \Sigma \phi_j$
			[VI]
			<u>Inert solute, no transformation</u>
			$\frac{\partial C}{\partial t} = D_S \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial z}$
			[VII]

Chemical Reactions

The last term (e) in equation 2 accounts for sources and sinks in the system, most being irreversible during the time period over which the equation is considered. The most common processes which are currently modeled are those of radioactive decay, chemical precipitation and dissolution, oxidation-reduction reactions, absorption of solutes by plant roots, and utilization and transformation of solutes by soil microorganisms. Except for radioactive decay, the terms ϕ_j are somewhat ambiguous and apply mainly to local conditions since the processes which are supposed to be modeled depend on very complex interrelationships of many physical and biological parameters incapable of being described without several empirical expressions and many simultaneous equations that often require numerical solution.

Sorption Models

The first term (a) of equation 2 describes the rate at which the solute interacts or exchanges with the solid phase. Its exact form continues to be heavily debated in literature. Both equilibrium and non-equilibrium assumptions are used when describing the adsorption-exchange processes.

Local Equilibrium Assumption (LEA)

Adsorption or exchange reactions perceived as instantaneous (as compared to the characteristic times of the dispersive (term (c) of equation 2) and the convective (term (d) of equation 2) processes) are described by equilibrium isotherms $S(C)$ which can be of different types (linear, Freundlich, Langmuir) or of many other functional forms (Bolt 1979).

It has been reported that these isotherms, being generally limited to narrow ranges of concentration, can take different values for adsorption as compared to desorption, especially for organic solutes (e.g. Van Genuchten et al. 1974, Calvet et al. 1980).

The most common approach for modeling the sorption term has been to assume a simple linearity between S and C :

$$S = K_d C \quad [3]$$

where K_d is often called the distribution coefficient.

Non-Local Equilibrium Assumption (NLEA)

In the past ten years laboratory and field investigations frequently revealed unexplained asymmetry or tailing of breakthrough curves, especially for sorbing solutes. Batch measurements of equilibrium sorption isotherms coupled with so-called traditional transport models have been found in many situations to be inadequate to explain these observations satisfactorily (see Valocchi 1985, table 1 for a review of experimental studies of solute transport in saturated soil columns).

A number of models have recently been proposed to predict such behavior. Their common premise is that non-equilibrium effects control the solute transport. These models can be grouped into two subcategories : chemical and physical non-equilibrium models.

Chemical non-equilibrium models. Chemically controlled kinetic rate reactions of the form $\partial S / \partial t = f(S, C)$ have been examined from various viewpoints. The most popular and simplest formulation arises when first-order linear kinetics is assumed (Lapidus and Amundson 1952) :

$$\frac{\partial S}{\partial t} = \alpha(KC - S) \quad [4]$$

where α is a first-order rate coefficient. Although this has led to some improvements in predictive capabilities of the models, success has generally been limited to experiments conducted at low pore water velocities (e.g. Davidson and Mc Dougal 1973, Van Genuchten et al. 1974).

An attractive chemical non-equilibrium submodel that did lead to improved transport descriptions is the two-site model: the basic idea is that the solid phase is made up of various constituents and that a chemical substance is likely to react with these constituents at different rates and with different intensities. Two types of adsorption sites are hypothesized: type-1 sites that achieve instantaneous equilibrium and type-2 sites with time-dependent kinetic adsorption. While adsorption on type-1 sites is described by

$$S_1 = FKC \quad [5a]$$

adsorption on type-2 sites is modeled by a linear first-order equation,

$$\frac{\partial S_2}{\partial t} = \alpha_1 [(1-F)KC - S_2] \quad [5b]$$

where F is the fraction of all sites that are type 1.

Physical non-equilibrium models. Non-equilibrium conditions have also been explained by diffusion-controlled sorption. Because of small particles and of vigorous shaking, diffusion can generally be eliminated as a rate-limiting factor in batch-type experiments. However, this situation does not necessarily occur in soils with flowing water where the sorption rate may be limited by the rate at which the ions are transported by diffusion to the exchange sites. This conceptualization has resulted in partitioning soil water in mobile (or flowing) and immobile (or stagnant) phases.

This leads us to consider a bimodal pore-water velocity: convective-dispersive transport is confined to a fraction of the liquid-filled pores and the remaining pores have stagnant water. This latter has been conceptualized as thin liquid films surrounding soil particles, as dead-end pores (Coats and Smith 1964), as non-moving intra-aggregate water (Philip 1968, Passouria 1971), or as isolated regions associated with unsaturated flow conditions (Nielsen and Biggar 1961). Transport models based on first-order exchange of solute between mobile and stagnant phases were initially presented in the petroleum (Coats and Smith 1964) and chemical engineering (Villermux and Van Swaay 1969) literature for non-adsorbing solutes and later extended to sorbing materials by Van Genuchten and Wierenga (1976).

The applicability of this concept to laboratory-scale transport processes has been clearly demonstrated for sorbing porous media (Van Genuchten and Wierenga 1977, Nkedi-Kizza et al. 1983, Van Eijkeren and Loch 1984, Jensen 1984, Carnahan and Remer 1984) as well as for a large variety of tracers (e.g. tritiated water and chloride) (Gaudet et al. 1977, Bolt 1979, De Smedt and Wierenga 1984).

Comparison of the two-site and two-region submodels shows that they have the same mathematical structure and they can be put in the same dimensionless form (Nkedi-Kizza et al. 1984). This similarity means that the two formulations can be used in a macroscopic and semi-empirical manner without having to define the exact physical and chemical processes which are involved at the microscopic level. It also means that independent experiments (such as batch studies and displacements with non reactive tracers) are needed for verification of the two phenomena.

Although two-region models may appear conceptually pleasing and have certainly resulted in improved prediction capabilities, the question remains whether or not they are too complicated for routine use in research and management. They require large numbers of parameters not easily determined, especially in field conditions. On the other hand, the more classical Fickian-based transport equation is much simpler and probably more attractive and suited for practical field applications.

Methods of Resolution

Numerous analytical, quasi-analytical and numerical solutions of equations 1 and 2 or of their equivalent and simplified forms have been presented in various recent publications (e.g. Addiscott and Wagenet 1985, Nielsen and al. 1986).

Analytical Solutions

In the analytical solutions of equation 1, the unsaturated soil properties and the initial and boundary conditions are suitably simplified or approximated such that exact or "quasi-analytical" solutions can be derived. While some of the solutions appear to be only of academic interest, others have or may prove to be useful for predicting unsaturated flow per se or for several indirect applications such as i) verification of numerical solutions (e.g. Vauclin et al. 1979), ii) formulation of approximate inverse problems leading to methods of determination of hydraulic properties, iii) derivation of physically-based equations for infiltration rates (e.g. Smith and Parlange 1978, Knight 1983, Haverkamp et al. 1988).

Many analytical solutions of the transport equation under steady-state water flow condition (equation VI of table 1) with and without sink terms are available (see Van Genuchten and Alves (1982) for an extensive review) for different types of initial and boundary conditions.

They have been used in studies on problems such as the influence of pore-water velocity on hydrodynamic dispersion, the interactions between leaching and solute adsorption, and ion exchange and solute transformations. Such solutions are useful because they permit great insight into the processes that can be incorporated and widely usable as long as the experiments they simulate meet the required boundary conditions. The latter constraint, however, has restricted their use mainly to carefully controlled laboratory columns of homogeneous and often destructured soils. Their validation in such experiments has probably given much credibility to their mechanistic aspect, but their practical use is greatly limited by the constraints of steady-state water flow and of boundary conditions needed for their development which rarely represent field conditions. It should be mentioned that approximate analytical solutions of equation V in table 1 have been recently proposed (Smiles et al. 1981, Bond and Smiles 1983) and successfully tested against experimental data (Bond 1986) for two sets of boundary conditions: constant water potential horizontal absorption and constant flux horizontal absorption.

Numerical Solutions

Solute leaching occurs in normal circumstances almost always under non-steady conditions for both water and solute. Appropriate formulations of equations 1 and 2 can then be simultaneously solved only by numerical methods (CSMP, finite difference, finite-element, and integrated finite difference techniques). Several such models are available for both one-dimensional and multidimensional problems.

The most important advantage of finite element techniques over standard finite difference methods is the ability to describe more accurately irregular system boundaries in multidimensional simulations as well as to take into account more easily nonhomogeneous medium properties. However, conflicting evidence still exists about the relative accuracy of finite-element versus finite difference techniques with respect to solution of the highly nonlinear flow equation (eq.1). It

should be noted that a good prediction of the solute distribution pattern requires an accurate estimation of the water flux.

As compared to analytical solutions, numerical models have proved very flexible in the range of initial and boundary conditions for both water and solute they can accommodate. They are able to avoid site-specificity by appropriate use of soil physical and chemical data. By developing more and more sophisticated numerical models the modelers, however should be aware that the real challenge remains that of an accurate characterization of relevant system parameters.

Limitations of The Approach

While the above deterministic and mechanistic models have been and will probably remain indispensable tools in research, several restraints to their practical use should be mentioned.

Parameter Identification

Both the analytical and numerical models require the knowledge of many parameters, the number of which depends on the degree of sophistication of the models themselves. Unfortunately, since several of these parameters are difficult to determine directly, they are often obtained by fitting the models to the test data through efficient optimization programs. While these methodologies may appear promising, they pose the problem of parameter uniqueness and introduce a semi-empirical character into the models.

Validation of The Models

The validity of the parameters identified by applying either analytical or numerical solutions is seldom checked against data other than those used in the identification procedure itself. When it is done, although the models basically simulate solute and/or water fluxes, they are generally tested against measured solute concentrations and/or water contents, which are not necessarily good indicators of fluxes through the vadose zone.

Field Applications of The Models

Further problems emerge when these models are used to describe solute leaching in the field, because of large uncertainties in the field experimental determination of the soil properties and of their spatial variation. For instance, field experiments have shown that the coefficients of variation for V and D_s may reach 400%! This casts doubt on predictive approaches based on the deterministic assumption that soil hydrodynamic properties can be described on a field scale, by single relationships between water flow velocity, water content and diffusion-dispersion. This recognition, coupled with experimental difficulties in the field determination of key parameters such as $K(\theta)$ and $D_s(V)$, has stimulated interest in other approaches briefly presented below.

DETERMINISTIC AND FUNCTIONAL MODELS

Addiscott and Wagenet's (1985) very detailed review remains current; we will therefore summarize its main features. Two classes of functional models may be considered: continuous and layer approaches.

Continuous Approaches

One of the easiest ways to simplify the theory governing solute movement is to compute the position of the solute peak by ignoring the effects of diffusion and dispersion. For instance, removing the dispersion term in equation V of table 1 reduces the equation to a piston flow

$$\theta \frac{\partial C}{\partial t} = -J_w \frac{\partial C}{\partial z}$$

The position α of the peak, defined by

$$\left. \frac{dC}{dz} \right|_{\alpha} = \frac{\partial C}{\partial z} + \frac{\partial C}{\partial t} \frac{\partial t}{\partial z} \bigg|_{\alpha} = 0$$

is then simply given by

$$\alpha = Q/\theta_{FC} \quad [6]$$

where Q is the amount of displacing solution and θ_{FC} is the soil field capacity.

In more sophisticated models (De Smedt and Wierenga 1978, Rose et al. 1982) diffusion and dispersion are taken into account, leading to compute the effects of these factors around the solute peak. For instance, by assuming an initially rectangular pulse (concentration C_0 , width ΔF), Rose et al. (1982) derived the following solution :

$$C/C_0 = 1/2 \left\{ \operatorname{erfc} \left[\frac{z - \alpha}{2(D_0 t + \lambda \alpha)^{1/2}} \right] - \operatorname{erfc} \left[\frac{z - \beta}{2(D_0 t + \lambda \beta)^{1/2}} \right] \right\} \quad [7]$$

where erfc = the complementary error function,
 D_0 = the molecular diffusion coefficient,
 λ = the dispersivity and
 β = $\alpha - \Delta F$ = the water penetration depth.

These partially analytical models are essentially capacity models since solute displacement is calculated using θ_{FC} and not rates of movement. They were designed to simulate the movement of a solute pulse and seem to do so with some success (see De Smedt and Wierenga 1978, for chloride concentrations; Rose et al. 1982, for ^{15}N -labelled N-fertilizer; Cameron and Wild 1982, for ^{36}Cl). It seems possible that they could also deal with successive pulses of solute by summing their effects. However, they seem to have potential limitations in that they are not able to simulate leaching in profiles which are heterogeneous or contain solute at the start of the leaching period. There do not appear to be any models of this "continuous approach" category that treat the problem of diffusion between mobile and less-mobile water. The need for λ , and to a lesser extent for D_0 , in equation 7 might also be a problem, but probably not a barrier to use. Also, only the Scotter (1978) model appears able to consider adsorbed solutes.

Layered Approaches

Chromatographic considerations (Reiniger and Bolt 1972, Villermanx 1981) have been used to simulate leaching in soils (e.g. Van der Molen 1956, Van Hoorn 1981). They offer great possibilities especially when multispecies transport is considered (e.g. Valocchi et al. 1981, Sardin et al. 1986), or reacting solutes are of concern (e.g. Frissel and Poelstra 1967); these topics remain relatively unexplored by soil physicists, soil chemists and hydrologists. In this approach soil is divided into horizontal layers (or cells) in which different chemical, physical and biological processes occurring simultaneously within each layer and between layers are considered. Mass conservation considerations in respect to both solute and water lead to algebraic equations that are fairly simple to solve. There are several such models, extensively reviewed by Addiscott and Wagenet (1985). Most of them calculate water flux from data on precipitation and evaporation, and one or two so-called characteristic moisture contents (field capacity, wilting point).

Examples of application are given by Bresler (1967), Tanji et al. (1972), Terkeltroub and Babcock (1971), Pandey and Gupta (1978) for salt leaching, by Burns (1974, 1980), Addiscott (1977, 1982) for nitrates.

Following a workshop held in March 1983 at the Institute for Soil Fertility in Haren, The Netherlands, with the aim of bringing together research workers in Western Europe who are designing and developing such layer models, De Willigen and Neeteson (1985) presented a comparison of six simulation models (Addiscott 1977, 1982, Burns 1974, 1975, 1976, Seligman and Van Keulen 1981, Richter et al. 1978, 1980, Van Veen and Frissel 1981, Zandt and De Willigen 1981) for the nitrogen cycle in the soil. All the models were run with the same data set, but not in all cases by the developers themselves (see table 1 of De Willigen and Neeteson paper). Although all the models gave a fair agreement between the dynamic behavior of the model output and the observations, Addiscott, Burns and Zandt-De Willigen models yielded the best results. However, all the results show that the main difficulties in modeling the soil nitrogen cycle lie in developing an adequate description of the microbiological transformations of nitrogen.

Apart from being mathematically simple, the models discussed in this section have the advantage that they require a limited number of data inputs, most of them obtainable without a prior fitting procedure. For field applications functional models based on capacity factors may present an advantage because these inputs appear less spatially-variable than rate parameters, provided they do not fail to simulate any important variability in real leaching. The Addiscott model was run with its inputs as single mean values and as probability distributions. The probability distributions yielded a slightly better simulation of field leaching data, but the difference was not large enough to suggest that omitting the variance of the inputs caused serious errors (Addiscott et al. 1986).

STOCHASTIC MODELS

It has been known for many years that local physicochemical properties in field soils can exhibit pronounced spatial fluctuations. The nature of this variability and the sampling problem it produces have been reviewed recently by Warrick and Nielsen (1980), Mc Bratney and Webster (1983), Vauclin (1983) and Peck (1983) among many others. This situation has led to the view that mass transport phenomena are intrinsically erratic processes susceptible to quantitative characterization by stochastic models. These models can be broadly categorized into i) approaches in which allowance is made for spatial variability of hydrodynamic soil properties in existing mechanistic models and ii) approaches focussed on the variability of solute and water movements through transfer functions, taking no account of mechanism.

Because very few such models will be analyzed in the second part of the paper, only a brief review is given here.

Stochastic and Mechanistic Models

In this type of model randomly-generated input values are used in a mechanistic model to produce a distribution of output values. While the stochastic behavior of water flow in the vadose zone has been relatively extensively studied (e.g. Warrick et al. 1977, Sharma and Luxmoore 1979, Warrick and Amoozegar-Fard 1979, Vauclin et al. 1983, Mantoglou and Gelhar 1987) few models deal with solute movement. Perhaps the best known representative of this approach is the model developed by Bresler and Dagan (1979, 1981, 1983).

The effects of regarding the field as a collection of uniform and homogeneous vertical soil columns differing only in their hydraulic properties, water and inert solute movements are described by equations III3b and V of table 1. If we apply the scaling hypothesis to these equations, the unsaturated hydraulic conductivity is viewed as a random stochastic process defined by a given probability density function of the scaling factors. This leads us to consider also capillary diffusivity, dispersion coefficient and water flux as stochastic processes. The resulting simulated spatial average (defined as the first moment of the probability density function) chloride concentration profiles were reasonably well related to measured ones, but the simulations were

poorer when the model was made deterministic by using a single scale factor. Wagenet and Rao (1983) were less successful when they attempted to simulate field-measured nitrate concentrations. This may be explained by the fact they worked on a cropped system with substantial solute and water extraction by roots.

Such models have given a conceptual framework for the development of further mechanism-based stochastic models and they have already proved useful for assessing the theoretical effect of variability. However, they make apparent the point that current use of stochastic concepts in subsurface solute-transport mechanistic theory should be considered as an initial attempt to capture and to model field scale variability in terms of a stochastic convective-dispersive equation. Many approximations now made in these models remain both untested in detailed field experiments and underived from rigorous results in the theory of random processes (see Sposito et al. 1986a or b for a discussion). For instance, the stochastic convective-dispersive model does not yet provide an analysis of the scale effect with a clear predictive value. It has not yet been applied to describe the transport of reactive solutes. It seems prudent to conclude that much more theoretical research is required before deciding whether this approach may be used as a tool for physically based, quantitative applications of solute transport theory to the management of solute movements at field scales.

Transfer Function Models

An interesting alternative approach, entirely non-mechanistic in form, lies in the transfer function model (TFM) suggested for soils by Raats (1978) and used by Jury (1982). The general, three-dimensional TFM was derived by Jury et al. (1986) from the principle of superposition and solute mass balance. Applying the TFM to a transport volume into which solute enters through one surface (entry surface) and from which it exits through a second surface (exit surface) the relationship between the entry $Q_{in}(t)$ and the exit $Q_{out}(t)$ mass flow rates is:

$$Q_{out}(t) = \int_0^t g(t-t' | t') Q_{in}(t') dt' \quad [8]$$

where $g(\tau | t')$ is the conditional solute lifetime density function, describing the probability that a solute molecule which enters the volume at t' leaves it between $\tau=t-t'$ and $\tau+d\tau$. It represents the lumped net effect of soil processes (e.g. convection, dispersion, sorption, radioactive decay, biological transformation) and modes of solute input on the lifetime of a solute in a unit of soil. Equation 8 may be expressed in terms of concentration to give:

$$C_{out}(t) = \int_0^t g(t-t' | t') i_{in}(t') C_{in}(t') / i_{out}(t) dt' \quad [9]$$

where $i(t)$ is the water flux.

For a steady-state water flow, the $i(t)$ in equation 9 cancel. In cases where the soil-water flux cannot be measured, Jury (1982) recommended an approximate TFM, in which the cumulative net applied water flux $I(t)$ was the dependent variable leading to replace equation 9 by:

$$C_{out}(I) = \int_0^I g(I-I' | I') C_{in}(I') dI' \quad [10]$$

This model was used successfully to describe transient solute outflow at different depths averaged over a 0.6-ha field by Jury and Stolzy (1982). Recently, White et al. (1986) and Sposito et al. (1986a or b) have provided additional insights into this stochastic convective approach by applying the TFM to some laboratory and field studies and by developing the two-component chemical and physical non-equilibrium convective-dispersive models as special cases of the generalized TFM.

It seems that this kind of model could be useful as a stochastically-based management model for solute movement, mainly because it requires a minimum of input data. However, it has the

disadvantages of all the transfer function-based models, classically used in hydrological processes e.g. the need for calibration, and the influence of the boundary conditions) and it is not yet known whether the approach will be satisfactory in vertically nonhomogeneous soils or whether it will give accurate estimates of flux as well as concentration.

A REVIEW OF SOME AVAILABLE MODELS

In order to make a proper evaluation of existing models a questionnaire was sent to 87 colleagues from 25 non-North American countries. The following information was requested:

- name and general purpose of model;
- type of model: deterministic (mechanistic/functional); stochastic (mechanistic/transfer function);
- modeled processes: convection, dispersion, adsorption, chemical reaction,...;
- soil (isotropic/anisotropic, homogeneous/heterogeneous, rigid/deformable, fractured system) and water flow (steady/transient, saturated/unsaturated, isothermal/non-isothermal) conditions;
- leachate nature;
- input data requirement (with method of determination of the parameters) and boundary condition type;
- model characteristics (solving technique, geometry of the domain, error criteria);
- model outputs (tables, graphics);
- program code information (language, computer make; code availability);
- model evaluation: check against theory ? applied to field or laboratory ? to other conditions than the one(s) on which the model has been validated;
- personal feelings about the strength(s) and the weakness(es) of the model and other models available in literature.

Thirty two answers were received. This relatively limited number makes the following analysis more informative than a real "state-of-the-art" review of models developed outside North America.

The models were categorized regarding their leachate nature rather than their type and characteristics. Three main domains with some interferences between them are covered by the survey : i) problems involving leachates other than nitrates, ii) problems involving the nitrogen cycle, and iii) problems dealing with multispecies transport, with chemical reactions.

Inert and Sorbing Leachate Models (nitrates excluded)

They represent 3 of the 32 models compared. The main characteristics and features of the models are summarized in table 2. Only model 5 is related to some extent to a continuous stochastic approach for solute transport.

All the others are either mechanistic (9) or functional (2). Most of the mechanistic models consider unsaturated transient vertical water flow described by either the Richards' equation or the Fokker-Planck equation (model refs. 4 and 8 in table 2). Only model 9 takes into account water uptake by roots. All the models except 9 and 11 assume the soil as isotropic, homogeneous along the profile and rigid. Models 9 and 11 are able to consider layered profiles characterized by different hydraulic conductivity and water retention curves.

In terms of solute transport, most of the models consider the local equilibrium assumption. Only 4 (refs. 2,3,6,8) consider mass exchange between stagnant and flowing water phases (two-region approach). All the models considering the adsorption process use the K_d approach, except model 9 which considers tabulated values of S versus C . Models 1 and 6 have options for considering different sorption isotherms (Freundlich, Langmuir).

Table 2.

Inert and Sorbing solutes: main characteristics of the models.

See Table 1 for the equation numbers. NLEA refers to physical non equilibrium submodels; CONV stands for convective transport.

Réf.n°	Authors	Model Name	Water flow	Solute transport	Leachate nature	Applications
1	Chardon (The Netherlands)	TRANS.CSM	Transient/saturated	Eq.IV no transf.	Heavy metals	Lab.
2	Dautrebande (Belgium)	-	Steady/unsaturated	Eq.V (NLEA)	tritium, pesticides	Lab.
3	Gaudet (France)	-	Eq.IIIa ($A=0$)	Eq.V (NLEA)	Cl^- , tritium	Lab.
4	Kirda et al. (Turkey USA)	-	Eq.IIIb ($A=0$)	Eq.VII	Cl^-	Lab.
5	Maciejewski (Poland)	SMMC	Eq.IIIa 2D ($A=0$)	Eq.V 2D	Cl^- , SO_4^-	Field/Lab.
6	Mermoud (Switzerland)	-	Eq.IIIa ($A=0$)	Eq.IV no transf. (NLEA)	not specified	
7	Nicholls (United Kingdom)	CALF	Layer approach	Eq.IV 1° order decay	Cl^- , pesticides, herbicides	Field/Lab.
8	De Smedt (Belgium)	TRANS	Eq.IIIb ($A=0$)	Eq.V (NLEA)	Cl^- , tracers	Lab.
9	Van Drecht (The Netherlands)	ONZAT	Eq.IIIa	Eqs.IV	Any chemicals	Field/Lab.
10	Vinten et al.	-	Layer approach	CONV	Total salt	Field
11	Vogel et al. (Czechoslovakia)	SIMP	Eq.IIIa ($A=0$)	Eqs.IV zéro + 1° order decay	Any chemicals	Field/Lab.
12	Zaradny (Poland)	SWATRZ	Eq.IIIa ($A=0$)	Eq.V	Cl^- , SO_4^-	Field/lab.

All the mechanistic models (except 1 and 2 which use CSMP and analytical solution respectively) are solved by the finite difference method, with a large variety of discretization schemes: explicit (model 4), fully implicit (3,5,9,12) and Crank-Nicolson (6,8,11).

In general information about the methods of determination of transport parameters is vague, if not absent. Precise information has been given in four answers dealing with laboratory experiments (3,4,6,8).

Five models are described as applicable to both laboratory and field conditions. In the latter case, not one considers the possible variability of transport coefficients and the parameters are taken from the literature or inferred by model calibration. Only four models (1,3,7,11) have been applied to conditions other than the ones on which they were developed.

N-Components Models

A similar analysis was made on the models intended to simulate nitrogen-component transport in the subsoil. Due to the practical importance of the problem in the agricultural world this item in our survey is the one in which the models are most oriented to field studies.

They account for 15 of the 32 surveyed. Their main characteristics and features are listed in table 3.

As in the previous case, a large variety of models have been found, from the simplest approaches (functional capacity-type) to the most elaborate ones (coupled transient water and solute transfers taking into account the fate of nitrogen in the vadose zone). In between, some models very similar to those considered above treat the transport of nitrates as a convective-dispersive process without any transformation.

References 14,15,16,20,25,26,27 are related to functional models. Models 13,17,19,21,24, belong to the mechanistic approach, all of them being numerical except ref.17 which analytically solves the water flow equation.

A very clear trend is seen in table 3: for field applications, only functional (layer-type) models, with simple description of the water flow component, are considered.

All the authors using this approach justify their choice by the fact that the hydraulic conductivity function is i) very difficult and time-consuming to determine, ii) too strongly nonlinear and too variable with water content, iii) subject to very large spatial variations. Therefore the estimates of water flux by using Darcy's law are too uncertain and erratic. One other unsaid, but essential point (in our opinion) is the following: high non-linearities in $K(\theta)$ and $\theta(h)$ curves impose such constraints in the discretization of equation 1, that time steps (typically from few seconds to one hour) are not compatible with available field data (daily values) and characteristic times of chemical processes such as mineralization/immobilization and nitrification/denitrification.

To justify the use of deterministic functional models at the field scale the authors generally argue (e.g. 14,20,24,25) that the capacity parameters are less variable than rate parameters. However, they recognize this as a possible weakness of this approach.

The assumption of steady-state water flow made in models (20,23,27) may present a strong limitation to their use under natural field conditions.

Transport models based on the two-region approach (14,16,19,21) seem to have potential application to structured soils with cracks and fissures.

Table 3.

Nitrogen cycle: main characteristics of the models. See table 1 for the equation numbers. HFE means that heat flow equation is considered. NLEA refers to physical non-equilibrium submodels, CONV stands for convective transport, PU stands for plant uptake.

Réf.n°	Authors	Model Name	Water flow	Solute transport	Leachate transf.	Applications
13	Ackerer (France)	None	Eq.IIIa + HFE	Eq.V + PU	Yes	None
14	Addiscott (U.K.)	SLIM	Layered	CONV (NLEA)	Yes	Field
15	Aslyng and Hansen (Denmark)	WATCROS /NITCROS	Layered + (AET, runoff)	CONV + PU	Yes	Field (production model)
16	Barracough (U.K.)	GAMON	Layered + AET	Eq.V (NLEA)	No	Field/Lab.
17	Clothier (New Zealand)	None	Analytical flux/conc.	Eq.VI	No	None
18	Geng et al. (France)	MORELN	Transient/sat. (2D)	CONV (2D)	Yes	Field
19	Huwe and van der Ploeg (W. Germany)	WHNSIM	Eq.IIIb + HFE	Eq.V (NLEA) + PU	Yes	Field
20	Kragt et al. (Holland)	RENLEM	Layered	CONV + PU	Yes	Field
21	Lafolie and Habib (France)	MONO	Eq.IIIa	Eq.V (NLEA) + PU	No	None
22	Merkel et al. (W. Germany)	GW-TR	not clear	Eqs.IV	Yes	Field/Lab.
23	Misra et al. (India USA)	None	Steady unsat./sat.	Eq.VI	Yes	None
24	Möller et al. (W. Germany)	SWACRO-M	Eq.IIIa (AET + runoff)	CONV	No	Field
25	Piehler (W. Germany)	EPIC (developed by WILLIAMS)	Layered (AET + runoff)	CONV	No	Field
26	Rijtema et al. (Holland)	ANIMO	Layered + HFE	CONV (O ₂ diffu.)	Yes	Field
27	DeWilligen and (Holland)	None	Layered	Eq.V	Yes	Field

Among the authors taking into account chemical nitrogen transformations (13,14,15,18,19,20,22,23,26,27) there is a consensus that the lack of an adequate description of the microbiological transformations represents a weakness of their model.

Models which do not consider transformations have also been addressed to other leachates than N-components: heavy metals for ref. 22, chloride for 14,16,17,22,24; sulfate for 22. Model SLIM (ref. 14) also simulates herbicides and pesticides movements in the vadose zone.

As in the previous case, the methods of parameter determination are not very clear in the survey. Generally speaking, the authors of functional models mention field and/or laboratory (undisturbed soil samples) determination of some key parameters such as capacity factors. On the other hand, authors of deterministic models use values taken from literature or estimated by curve-fitting procedures applied to observations, generally obtained on well-defined and controlled experiments conducted on soil columns, and numerical results. Due to the large number of parameters the uniqueness of the results may pose problems that are not really mentioned in the survey.

Multispecies Transport Models

This class of the chemical-oriented models deals with transport of solute taking into account such chemical reactions as ion-exchange, precipitation/dissolution, and complexation. The five models reviewed in the survey (see table 4) are deterministic, the first four being mechanistic, the last one resulting from chromatographic considerations.

All the models accommodate multiple ion transport. Model 30 is surely the most sophisticated, since the transient transport equation, apart from describing the convective and dispersive processes, includes optional submodels for different chemical phenomena (ion exchange, complexation, precipitation, dissolution, and carbonate fate), plant uptake of cations, and oxygen transport and consumption. It is coupled with the water flow calculated by the SHE model (Système Hydrologique Européen; see Abbott et al. 1986).

SIMUL (ref. 31) appears to be one of the rare models which has been successfully used at the field scale by persons (in Tunisia and Brazil) other than the author for studying soil salinity hazards. The model is based on the numerical solution (implicit finite difference scheme) of the Fokker-Planck equation coupled with convective transport of solutes considering precipitation (for calcite and gypsum), and ion exchange (for Ca, Na and/or Mg) processes. All the thermodynamic equilibrium calculations are based on the studies performed by Laudelout et al. (1979).

Table 4.
Multispecies transport models: main characteristics. See table 1 for the equation numbers. CHEM stands for chemical reactions.

Réf.n°	Authors	Model Name	Water flow	Solute transport	Leachate nature	Applications
28	Chen and Li (People's Rep. of China)	MITM	Not specified	Eq.VI	Cl^- , SO_4^{--} , Ca^{++} , Na^{++} , Mg^{++}	None
29	Pachepski et al. (USSR)	FAUST	Not specified	Eq.VI	Cl^- , SO_4^{--} , Na^+ , Ca^{++} , Mg^{++} , HCO_3	Lab.
30	Refsgaard and Ammentorp (Denmark)	None	Eq.IIIa(SHE model)	Eq.VI (NLEA)	Any	Field/Lab.
31	Rieu (France)	SIMUL	Eq.IIIb (AET)	CONV + CHEM (Layered)	Cl^- , SO_4^{--} , Na^+ , Ca^{++} , Mg^{++}	Field/Lab.
32	Schweich et al. (France)	IMPACT	Steady sat./unsat.	Eq.VI (layered)	Any	Field/Lab.

Model IMPACT (ref. 32) is based on chemical engineering concepts. The water flow is estimated through the residence time distribution. The transport equation, based on convective and dispersive processes, is able to account for any mass action law for any chemical. The authors rightly mention the danger of blindly using the K_d approach to model the mass exchanges between solid and solution phases. The assumption of steady-state water flow regime seems to be one of the most important limitation to the use of the model under field situations.

The other models (refs. 28 and 29) can be considered as geochemical ones. In the light of the information given by the authors, it has not been possible to determine whether the water flow is assumed to be known or is really calculated.

For this class of models more information has recently been provided by Engesgaard and Christensen (1988) who extensively review 19 other chemical solute transport models; among them 8 deal with the unsaturated zone.

Discussion

From this review it is possible to draw some general conclusions about the state of the art of transport models. It is clear that this selection (it has not been made by the reviewers, but is based only on the survey responses) of models shows great diversity with respect to complexity and general applicability to field-scale problems. This conclusion is based on the fact that many of the models are developed for a specific purpose and thus are as complex as needed.

Some of the models cannot be used elsewhere where assumptions on which they are based are violated. It has therefore been difficult to point out models which are formulated in such a general way that they can be applied to almost any system.

Analytical solutions of the mechanistically-based convection-dispersion equation are soundly based and have been validated in carefully controlled laboratory experiments. However their deterministic nature as well as their specific initial and boundary conditions limit their use to experiments designed around them. They are mainly research models and tools for parameter identification.

Numerical models based on this equation are more flexible than the analytical ones and therefore able to simulate transient solute movement in the field, but their deterministic nature makes them of questionable use because of the spatial variability and local uncertainties of soil hydraulic properties. The large number of input parameters as well as small time and space steps of calculation constitute other constraints to their practical use. These models also tend to be oriented toward research.

Stochastic models developed to take into account the variability of hydraulic properties have proved useful for assessing the theoretical effect of this variability. Although appearing as research models at present, some of them have potential for management purposes.

Functional, less-mechanistic models have modest input data requirements, most of them being obtainable independently of the test data. A typical time step of calculation is one day. This makes them potentially well-adapted for management purposes. However, their reliance on capacity-type soil water inputs could result in failure to simulate variation in leaching (including upward fluxes) that is of practical importance.

CONCLUDING REMARKS

The field of solute transport modeling is in the midst of an exciting period of growth and challenge. Various reviews published in recent years have revealed progress in many areas.

Investigators have uncovered a number of inadequacies with existing models of soil transport processes and have made significant steps toward a better understanding of these phenomena. Some new research areas such as biodegradation modeling, immiscible phase transport, water and solute transfers in structured or swelling soils, and multi-interactive ion transport are emerging.

A number of challenges still remain for both the theoretician and the practitioners. They include

- i) how best to deal with preferential water flow and transport,
- ii) how best to model the effects of local and regional spatial and temporal variabilities of soil hydraulic properties on solute transport,
- iii) how to couple multi-component geochemical submodels efficiently with available unsaturated-saturated flow models,
- iv) how to improve field methods for estimating vadose zone transport parameters and
- v) how best to predict the long-term consequences of short-term management decisions.

It is apparent that the complexity and variety of the physical processes have led to increasing specialization within the area of transport modeling. Soil physicists, soils chemists and soil microbiologists have the propensity to limit their consideration and vision to their respective disciplines. For example, soil physicists still tend to disregard the chemical interactions between solid and solutes by neglecting terms (a) and (e) in equation 2, utilize solutes to evaluate the behavior of D_s for different water flow regimes and suggest improvement in the formulation of similar equations based, for instance, on geometrical considerations of the soil pores. Soil chemists emphasize mechanisms and parameters involved in terms (a) and (e) in equation 2 at the expense of the physical aspects of the system (terms (c) and (d)). Soil microbiologists mainly study the last term of equation 2 in relation to the growth and maintenance of microbial population and very often choose experimental conditions so that terms (c) and (d) are neglected.

A natural consequence of this specialization has been the evolution of scientific jargon specific to each subdiscipline. This may be overcome by reinforcing interdisciplinary cooperation among investigators, by training of students both at the graduate and postgraduate levels and by encouraging topical workshops and publications in interdisciplinary journals. The effort being made in Europe through multidisciplinary research programs supported by European Communities (DG XII) in the domain of Environment and Soil quality should be highly rewarding in that sense.

Another general observation gleaned from this review is that very few solute transport models have been exhaustively tested under field conditions. Indeed, the quantitative criteria for validating models do not seem to be clearly identified or universally recognized. It appears very important that such criteria should be established and used to make an objective comparison of the abilities of the various types of model to simulate the results of field experiments. Without such tests and without comparisons between models there is a risk that disagreements between the predictions of different models and the resulting confusion could greatly diminish the usefulness of modeling techniques. While computer codes escalate in number as pressures mount for improved management strategies it is time for asking the question: should the scientific community continue to develop more and more sophisticated general or even specific models or should it put an emphasis on field experiments? Obtaining an answer will probably be of great importance in the near future. As a matter of fact, because of decreasing computer costs and relative increase in the cost of carefully designed field experiments, there is a worldwide trend to "observe the water and solute movements through computer screens"! The modelers should be aware that without reliable estimates of the input parameters as well as in-situ validation their models will appear more as intellectual games of academic interest rather than as tools to help the practitioners in their management decisions.

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LEACHING MODELS OF THE UNSATURATED ZONE: THEIR POTENTIAL USE FOR MANAGEMENT AND PLANNING

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"Thus one can think of the unsaturated zone as a pollutant-filled time bomb, which ticks slowly, but which will eventually explode." (Goldshmid, 1984)

ABSTRACT

This paper gives a review of models in use outside the USA dealing with leaching of pollutants in the unsaturated zone. An inventory of such models is presented in a table. It is concluded that only a few are suitable as such for application in management and planning. Three case studies pertaining to leaching of nitrate, phosphate and herbicides are discussed.

INTRODUCTION

Input of fertilizers and pesticides can be a highly effective means to increase crop yields. Unfortunately, the increasing use of agrochemicals has also created environmental problems of which degraded water quality is considered one of the most serious. Fertilizers or heavy metals not taken up, or pesticides not volatilized or decomposed are potential pollutants of groundwater. Before any such pollutant can reach the groundwater it has to pass through the unsaturated (vadose) zone, which can be said to be "the buffer between human activity and the groundwater sources" (Goldshmid 1984). In order to control agricultural pollution, a better quantitative understanding is needed of the effects of different soils, climatic conditions and combination of crops on the cycling of agrochemicals in, and leaching out of, the vadose zone. Therefore, interest in using mathematical models has rapidly increased, for the purpose of analyzing the behavior of water and chemicals in agricultural soils, and for policy evaluation and management.

A large number of nonpoint-source models have been devised and are available for planners dealing with agriculture and water quality (see table 1 and reviews by Frissel and Van Veen 1981, Haith 1982). The differences between these models usually concern structure, underlying assumptions and general purpose. The complexity can range from relatively simple models of solute transport which are used for estimating fertilizer movement (Burns and Greenwood 1982) and for making regional estimates of leaching losses (Burns and Greenwood 1982; Bergström et al. 1987) to more comprehensive models used as research tools (Van Veen and Frissel 1981). The simpler, empirically-based models are more suited for widespread use since they require considerably fewer input data than complex, multi-process models. However, a number of complex models have also been developed with a view to widespread application (Johnsson et al. 1987). The applicability of a model is more often limited by the need for calibration rather than by complexity, since models requiring calibration have limited use for sites which lack monitoring programs.

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This paper summarizes and discusses model characteristics of interest to potential users, and presents a state-of-the-art review of experience with leaching models developed outside the USA. Case histories of a selection of leaching models dealing with nitrogen, phosphorus, and pesticides are presented.

AVAILABLE NONPOINT-SOURCE MODELS

A list of leaching models in use outside the USA is presented in table 1. This list is based on information collected by Vachaud et al. (1988). Although all are intended for leaching problems, the models listed are quite different in terms of complexity and general purpose.

The majority of the models (18 of 29) deal with linearly-adsorbed or nonadsorbed pollutants. Because the classical convection-dispersion transport equation (see equation 1 below) with steady flow and linear production/consumption term applies here, many analytical solutions are known, for widely divergent boundary conditions. Van Genuchten and Alves (1982) made a catalogue of such solutions. In addition to nonsteady flow, an important reason for solving the equation numerically is the fact that the production/consumption term is nonlinear and/or is a complicated function of environmental conditions (temperature, water content). Most of the nitrate leaching models include a description of nitrogen transformations (mineralization, (de)nitrification).

Nonlinear adsorption is considered in two models (ONZAT, and model 10), one (ONZAT) treating generally nonlinearly sorbed solutes, whereas the other specifically deals with cadmium. Ion exchange is included also in two models (MITM and IMPACT). Such models are particularly intended for use in descriptions of transport of cations (e.g. Ca, Mg, and K).

The models previously mentioned assume that instantaneous chemical equilibrium exists. Nonequilibrium in adsorption or in other chemical reactions is taken into account in the models dealing with phosphate (models 14 and 27) and pesticides (models 8 and 21).

The major transport mechanism for pollutants is transport with water. Leaching in a field situation generally occurs under nonsteady conditions, and flow of water for such circumstances should in principle be calculated fundamentally, i.e., using Richards' equation. This is usually quite time-consuming, and does not necessarily lead to better results as far as solute leaching is concerned (Wierenga (1977), Richter et al. (1978), Beese and Wierenga (1980), De Willigen and Neeteson (1984)). Of the models in table 1, 11 solve Richards' equation; the others either describe time-variable waterflow in a simplified way, or assume steady conditions. Five models partition the soil water into mobile and immobile parts; transport is limited to the mobile part only, whereas there is an exchange of solute between the mobile and immobile parts. As shown by Nkedi-Kizza et al. (1984), this description is equivalent to that where chemical nonequilibrium is considered.

Only one model deals with spatial variability (model 28), but it should be mentioned that De Haan et al. (1987) and Van der Zee and Van Riemsdijk (1987) considered spatial variability of cadmium sorption parameters using a simplified version of model 10.

Few of the models are at present suitable for solving problems related to management and regulation. Of the 29 models listed in table 1, only two were specifically designed for management purposes: PULSE (Bergström, 1987) and MORELN (Geng et al., pers. commun.). Model 24 was originally set up as a simple transport model for nitrate, but has evolved into a model for the complete nitrogen regime, to be used for advisory purposes. As opposed to the situation in the USA, in Europe and elsewhere little emphasis has been put on the development of management-oriented models. However, simulation models designed primarily for research in principle do have the potential to be used for management and planning. One of the reasons for the limited practical use of such models is the lack of thorough validation of the models. Sixteen

of the models in table 1 have been validated against field data; still fewer (viz. 13) have been used for sites other than those for which they were originally validated. Moreover, in many cases too many site-specific parameters are used that are not readily available or very difficult to obtain. In order for models to be used as management tools, a prerequisite is that proper documentation is available and that the model code is easy to understand for users other than the model designer. Only about one third of the models cited in table 1, can, in the opinion of their designers, be used without author supervision or advice. As one tends to overrate the lucidity of one's own work, this is probably an overestimation of the accessibility of these models.

Table 1. List of leaching models discussed in this paper.

Model name	Authors	Country	Pollutant	Remarks
1.SLIM	Addiscott,T.M.	UK	Nitrate	Mobile/immobile phases
2._____	Ackerer,P. 1/	France	Nitrate	Major N-transformations, plant uptake, heat transport
3._____	Ammentorp,H.C. Refsgaard,J.C.	Denmark	Any ions	Ion exchange, oxygen transport (1988)
4.NITCROS	Aslyng,H.C. Hansen,S. (1984)	Denmark	Nitrate	Major N-transformations, plant uptake
5.GAMON	Barraclough,D. (1988)	UK	Nitrate	Mobile/immobile phases
6.ANIMO	Berghuijs,J.T. Rijtema, P.E. Roest,C.W.J (1985)	Netherlands	Nitrogen	N-transformations, oxygen demand, heat transport
7.PULSE	Bergström,S. Brandt,M. Gustafson,A. (1987)	Sweden	Nitrate	Major N-transformations, plant uptake
8._____	Boesten,J.J.T.I (1986)	Netherlands	Pesticides	Instantaneous and time-dependent adsorption and decay
9._____	Burns,I. (1975)	UK	Nitrate	
10.TRANS.CSM	Chardon,W.J. (1984)	Netherlands	Cadmium	Nonlinear adsorption

1/ no publication available, see list of addresses

Table 1. continued.

Model name	Authors	Country	Pollutant	Remarks
11.MITM	Chen,W., 1/ Li, I.	China	Any ions	Ion exchange
12. _____	Dautrebande,S. (1985)	Belgium	Linearly adsorbed solutes	Mobile/immobile phases, originally developed by Van Genuchten & Dalton (1986).
13.TRANS	De Smedt,F. Wierenga,P.J. Van der Beken,A. (1981)	Belgium	Linearly adsorbed solutes	Mobile/immobile phases
14. _____	De Willigen,P. Raats,P.A.C. Gerritse, R.G. (1982)	Netherlands	Phosphate	Instantaneous adsorption, time- dependent fixation
15. _____	Ferrari,Th. Cuperus,J.L. (1973)	Netherlands	Nitrate	
16.MORELN	Geng,Q.Z. Girard,G. Ledoux,E. (1987)	France	Nitrate	Major N-transformations, management- oriented
17.SOILN	Johnsson,H. Bergström,L. Jansson,P.-E. Paustian,K. (1987)	Sweden	Nitrate	Major N-transformations, heat transport
18. _____	Kirda,C. Nielsen,D.R. Biggar,J.W. (1973)	Turkey	Chloride	
19.MONO	Lafolie,F. 1/ Habib,R.	France	Nitrate	Mobile/immobile phases, plant uptake
20a.SWATRZ 20b.SMMC	Maciejewski,S. 1/ Zaradny,H.	Poland	Linearly- adsorbed solutes	SMMC considers two-dimensional transport

1/ no publication available, see list of addresses

Table 1. continued.

Model name	Authors	Country	Pollutant	Remarks
21.CALF	Nicholls,P.H. Walker,A. Walker,R.J. (1982)	UK	Pesticides	
22.FAUST	Pachepski,J.A. Mironenko,E.V. Ponizovski,A.A. (1988)	USSR	Any ions	Ion exchange
23.EPIC	Piehler,H.	BRD	Nitrate	Includes erosion originally developed by Williams et al. (1983).
24._____	Richter,J. Kersebaum,K.Chr. Utermann,J. (1988)	BRD	Nitrate	
25.IMPACT	Schweich,D. Sardin,M. Jauzein,M. (Sardin et al., 1986)	France	Any ions	Non-linear adsorption
26.ONZAT	Van Drecht,G. (1986)	Netherlands	Non-linear adsorbed solutes	
27._____	Van Der Zee,S. Van Riemsdijk,W.H. (1986)	Netherlands	Phosphate	Non-linear adsorption, time dependent fixation considers spatial variability
28.SIMP	Vogel,T.1/ Cislerova,M. Simunek,J.	CSSR	Linearly adsorbed solutes	
29._____	Zandt, P.A. Willigen, P.de (1981)	Netherlands	Nitrate	Includes major N-transformations

1/ no publication available, see list of addresses

CASE STUDIES

From the models listed in table 1, we selected three models dealing with leaching of nitrate, pesticides and phosphate, respectively, which we will discuss in case studies. The models are well documented, have been tested and validated against field data, and are suitable for use in management, regulation and planning.

General Transport Equation

All models discussed in this section numerically or analytically solve the general one-dimensional equation of transport by diffusion/dispersion and convection:

$$\frac{\partial}{\partial t} (\rho F + \theta c) = \frac{\partial}{\partial z} D \frac{\partial c}{\partial z} - \frac{\partial}{\partial z} v c + S \quad [1]$$

where ρ = the bulk density of the soil [ML^{-3}],
 F = the amount of sorbed pollutant per unit soil mass [1],
 θ = the volumetric water content [1],
 c = the concentration of the pollutant in the soil solution [ML^{-3}],
 D = the diffusion/dispersion coefficient [L^2T^{-1}],
 v = the flux of the soil solution [LT^{-1}],
 z = the vertical coordinate [L], and
 S = the production/consumption of the pollutant in the soil [$\text{ML}^{-3}\text{T}^{-1}$].

It is assumed that transport only takes place in the liquid phase.

Case Study 1: Leaching of Nitrogen

Models dealing with nitrate leaching and nitrogen transformations in agricultural soils vary widely in scope, but their main structures usually show distinct similarities. The biological, chemical, and physical processes included in these models are either described in a mechanistic way or by empirically-based relations. Quite often combinations of the two also occur. In the model chosen for the case histories described here (SOILN, see table 1) both mechanistic and empirically-based submodels are included (Johnsson et al. 1987). This model was applied to several sites and data sets: sites where the information on processes included was extensive (Johnsson et al. 1987; Bergström and Johnsson 1988), and data sets describing relatively long-time series, comprising several crops (Jansson et al. 1987, Gustafson 1988). It has also been used to evaluate long-term trends in nitrate leaching in a whole watershed where information was very sparse (Jansson and Andersson 1988). These various applications, with completely different prerequisites concerning input data, suggest that relatively comprehensive models can also be useful for applications-oriented problems related to planning, management and regulation.

Only an overview of model structure and basic assumptions underlying important processes are given here.

Structure of the Model

The model consists of two parts which are used in sequence. First, soil moisture and temperature conditions are simulated in a water and heat submodel. Its outputs are utilized as driving variables for the nitrogen submodel. Common to both submodels is the vertical structure that facilitates division of the soil into different layers depending on the resolution requested and information available on basic physical and biological characteristics.

Water and Heat Transport

The water and heat submodel has been described earlier by Jansson and Halldin (1980). It is based on two coupled differential equations describing heat and water transport (derived from Fourier's and Darcy's laws, respectively) in a one-dimensional soil profile. Snow dynamics, frost, evapotranspiration, precipitation, groundwater flow, water uptake by the plant, and drainage flow are included. The model predicts daily values for soil temperature and soil water content at any level in the soil profile using standard meteorological data as driving variables.

The model also deals with water transport in the saturated zone. The flow rate from each saturated layer above the depth of the drainage tiles is calculated, taking into account the thickness of the layer, the saturated conductivity, the depth of the drainage tiles, the depth of the groundwater table and the distance between drainage tiles. In addition to the water flow drained via the drainage tiles, the saturated water flow directed toward a stream or ditch is calculated with an empirical equation.

Surface runoff can occur due to limited infiltration capacity or limited permeability of the soil.

Nitrogen Transformations and Plant N-Uptake

A detailed description of the nitrogen model is given by Johnsson et al. (1987). Biological N-transformations in the model (fig. 1) apply to each layer. Mineral-N pools include ammonium and nitrate. Organic-N is distributed over litter, feces, and humus. The carbon pools for litter and feces are included to control nitrogen mineralization and immobilization rates. Undecomposed material (e.g., crop residues, dead roots, microbial biomass) constitutes the litter component, while the humus component consists of stabilized decomposition products.

Mineralization of humus-N (denoted as N_h) is calculated as a first-order rate process:

$$N_{h \rightarrow NH_4} = k_h e_t e_m N_h \quad [2]$$

where k_h = the specific mineralization constant [T^{-1}],
 e = response function, subscripted to denote temperature and moisture [1], and
 N_h = the mass of humus-N [M].

Similarly, decomposition of the organic carbon pools of litter and feces are calculated as first-order rate processes controlled by specific mineralization constants and by response functions for soil moisture and temperature (the same as those used for mineralization of humus-N). Of the decomposed carbon in the litter and feces pools, one fraction ($1-f_e$) is lost to the atmosphere as CO_2 , the fraction $f_e(1-f_h)$ is recycled within the pools, and the fraction $f_e f_h$ is stabilized as humus. The parameters f_e and f_h represent an efficiency constant and a humification fraction, respectively. Corresponding nitrogen flows are calculated assuming a constant C/N ratio of decomposing biomass and humification products (r_o). The net mineralization or immobilization in the litter pool is calculated as:

$$N_{l \rightarrow NH_4} = (N_l/C_l - f_e/r_o)C_{ld} \quad [3]$$

where N_l and C_l are the masses of nitrogen and carbon in the litter pool, and C_{ld} is the decomposition rate of litter carbon. The same equation is valid for the feces pool. When net immobilization occurs (i.e., $N_l/C_l < f_e/r_o$) the immobilization is limited to a maximum available fraction in the soil. Both ammonium and nitrate can be immobilized, with preference for available ammonium.

Nitrification of ammonium to nitrate is calculated from the excess of ammonium present when the ammonium/nitrate ratio exceeds an assumed equilibrium. The calculation employs a specific rate constant and abiotic response functions.

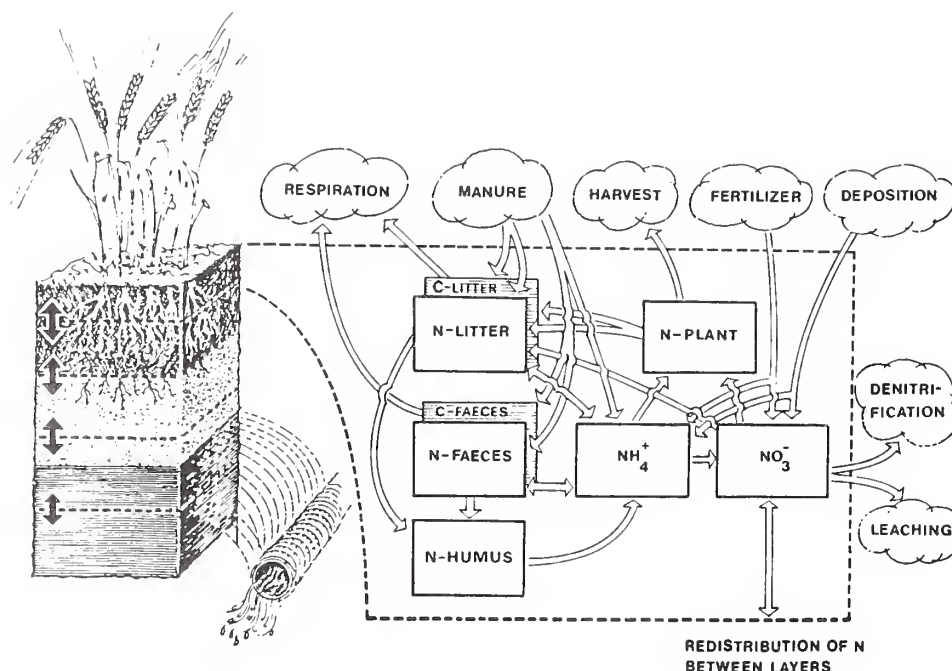


Figure 1.
Structure of the nitrogen model (SOILN). Components within the dotted line represent the uppermost soil layer. Subsurface layers have the same structure but do not receive any direct inputs from fertilizer and deposition (from Johnsson et al. 1987).

The abiotic response functions regulating decomposition, mineralization, and nitrification are functions of soil temperature and soil water content. An exponential expression is used for temperature, where the response increases by a factor 2 for a rise in temperature of 10°C. An empirical relationship is used for volumetric water content, based on the assumption that the range within which water content is optimum is defined by two thresholds representing dry and very wet soil.

Denitrification is calculated as a zero-order process based on a potential rate and on response functions of temperature, water content, and nitrate concentration. The temperature response function is the same as that used for other microbial processes, while the response to water content is zero up to a value close to saturation, from where the response increases with increased water content to an optimum level at saturation. The nitrate concentration response is calculated with a Michaelis-Menten expression with a half-saturation constant (cf Burns 1978).

Plant uptake of nitrogen is controlled by an assumed root distribution and a potential logistic growth curve. Nitrogen uptake is reduced when the demand exceeds a maximum availability fraction of mineral-N in the soil, similar to the situation described for immobilization. The ratio of ammonium uptake to nitrate uptake was taken to be the same as the ratio of ammonium to nitrate in the soil solution.

Agricultural management characteristics and different crop characteristics can be used to estimate most model parameters controlling inputs and outputs of nitrogen. The most important information requirements for determining model parameters are those describing different nitrogen transformations in the soil. Some of the parameters are well known from laboratory studies while others are only qualitatively known and have to be estimated (Johnsson et al. 1987)

Transport of Nitrogen

Only nitrate is considered to be mobile, and nitrate flows are calculated as the product of water flow and nitrate concentration in the soil layer from which the water flow originates. Diffusion and dispersion are not explicitly accounted for, but due to the division of the soil profile into layers of finite thickness, numerical dispersion sometimes occurs.

Site Description

To test the applicability of the model to different field data sets, two extreme applications concerning available information for validation of the various parts of the model were chosen.

First, the model was applied to a field for which extremely detailed information was available. This field in central Sweden, Kjettslinge, was the experimental site for the project "Ecology of Arable Land" (Persson and Rosswall 1983, Steen et al. 1984). Data were collected on decomposition, denitrification, leaching, mineralization, mineral-N profiles, primary production, and soil abiotic conditions. The climate is cold-temperate and humid with annual precipitation of 520 mm and mean annual temperature of and 5°C. The topsoil, 30-cm thick, contains 15-20% clay, 2.2% organic carbon and has a pH of 6.0-6.5. The topsoil is underlain by a layer of fine sand with average thickness of 25 cm, underlain by an oxidized clay layer down to a depth of about 75 cm, and finally an non-oxidized clay layer down to 100 cm. Simulated and measured nitrate leaching and mineral-N profiles were compared in two treatments with barley (with and without N-fertilization (120 kg N/(ha·yr)) (Johnsson et al. 1987) and a fertilized (200 kg N/(ha·yr)) grass ley (Bergström and Johnsson 1988). The simulated periods were 3 and 4 years, respectively, on each 0.36-ha plot size.

Secondly, the model was tested on a 202-km² watershed in southern Sweden. Simulated values of nitrate leaching were compared with measurements for a 20-year period (Jansson and Andersson 1988). More than 2/3 of the total flow of nitrogen in the river draining the basin originated from agricultural nonpoint sources (Andersson 1986). The proportion of the area under perennial leys decreased from 16 to 3% during the 20-year period, whereas that under cereals increased from 44 to 57%. On the remaining part sugar beets and oilseed rape were grown. The predominant soil type in the area is clay till with a well-developed structure, well aerated, and with favorable water-holding characteristics. In the simulation, a grain field was chosen to represent arable land in the area. Most of the parameter values in this application had to be estimated from the literature or from agricultural statistics for the region. This, in combination with the problems of analyzing field measurements from watersheds integrating many biologically and physically different subareas, made a detailed analysis of the simulated results difficult.

Results

The main objectives of the simulations with Kjettslinge data were to obtain a thorough test of the different model components and to evaluate the usefulness of the model for studying nitrate leaching in annual and perennial crops. In the watershed simulation, efforts were made to elucidate trends in nitrate leaching over the 20-year period as indicated by measurements. The relative importance of labile and stable organic matter (litter and humus) in supplying mineral N to the soil and thus affecting leaching losses, was tested. Therefore, two sets of parameters were used, one representing a fast turnover of organic matter (because the major part of the litter-N was assumed to move directly to the soil) and one in which litter-N was largely directed to the humus pool, representing a slow turnover of organic matter.

The detailed field simulation. Since simulation of nitrate leaching depends on model output both of nitrate concentration and of drainage water flow, three time series of cumulative leaching were compared: (1) calculated from measured nitrate concentrations and simulated drainage (i.e., "partly simulated") (2) calculated from simulation of both nitrate concentrations and drainage flow, and (3) measured. Figure 2 shows this comparison. In this way deviations in leaching pattern caused by

either poor predictions of drainage water flows or of nitrate levels could be isolated; however, this was only done in the simulations with barley as test crop. Cumulative nitrate leaching was similar in all time series. The greatest differences between measurements and simulations occurred during the initial year (1981) and were largely due to underestimated drainage water flows in the simulations.

Similar results were obtained for the grass ley, as shown in figure 3. In this case a substantial difference between simulated and measured nitrate leaching also occurred at the end of 1984; in this case, the reason can also be found in deviations in drainage behavior. The earlier start and short duration of measured drainage and leaching at the end of 1984, compared with the corresponding simulated values, can be accounted for by soil physical conditions. Macropore flow and lateral water flow in layers with high hydraulic conductivity are the most plausible causes of the earlier start. Once vertical flow becomes dominant in the field, the groundwater table, which had fallen considerably during the dry years 1982 and 1983 (Alvenäs et al. 1986), had to rise again before any water flow through the drainage tiles could be expected. This explains the absence of measurable nitrate leaching after the initial, rapid tile-drainage flow. Neither flow through macropores in dry soil directly to drainage tiles nor lateral water flow above the groundwater table are considered in the model, which explains the discrepancy between simulated and measured nitrate leaching in the grass ley during 1984. In that year, however, simulated leaching was in good agreement with measurements in lysimeters at the Kjettslinge field (Bergström 1987) in which percolation to deeper groundwater did not occur. This test indicates that the model considerably underestimates nitrate leaching from tile-drained plots.

In both simulations with Kjettslinge data the nitrogen part of the model was adapted to obtain reasonable agreement between simulated and measured values for soil mineral-N content. The simulated values for nitrate leaching were arrived at independently. The fairly good agreement between simulated and measured values of leaching in these two Kjettslinge applications indicates that good leaching predictions can be obtained with a simulation model if data on soil mineral-N content are available (cf. Jansson et al. 1987).

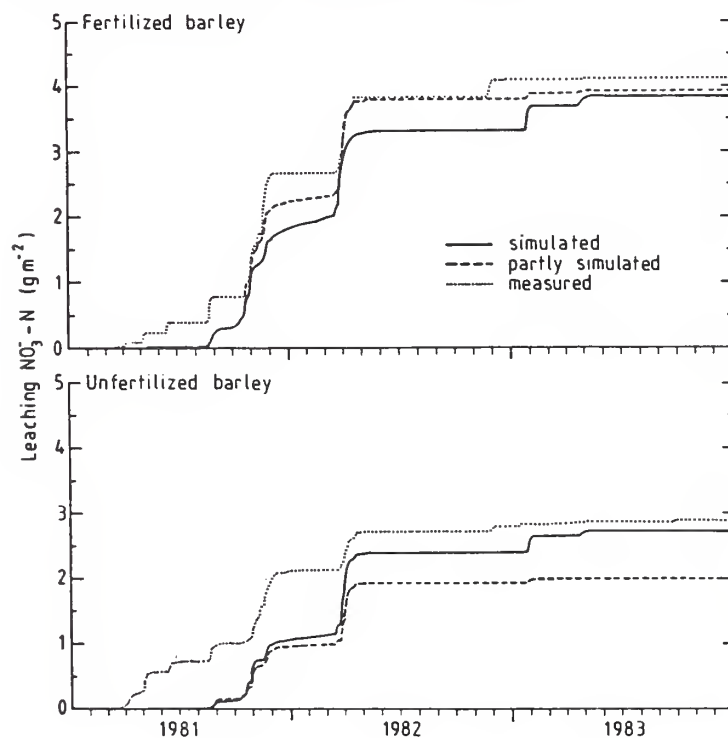


Figure 2. Simulated, "partly" simulated, and measured cumulative nitrate leaching from the barley crops at Kjettslinge (from Johnsson et al. 1987).

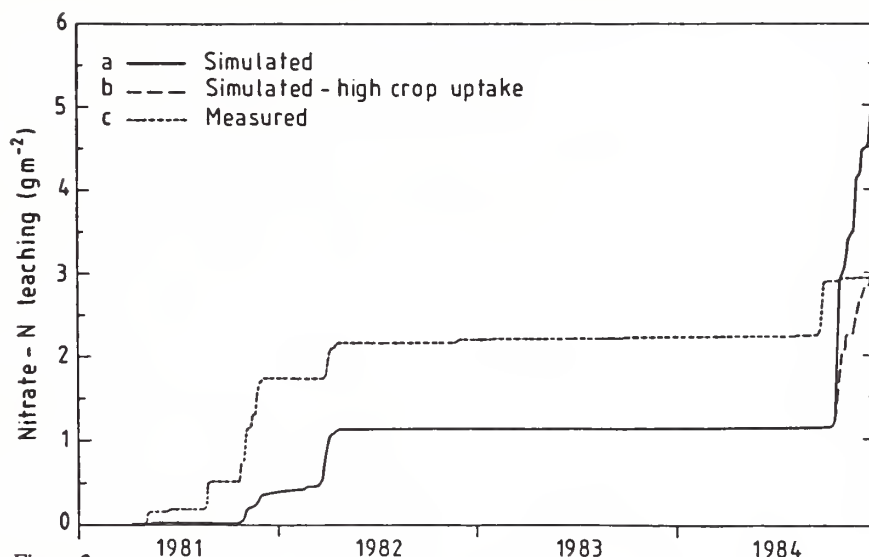


Figure 3.
Simulated and measured cumulative nitrate leaching from the grass ley
at Kjettslinge (From Bergström and Johnsson 1988).

The watershed simulation. Over the 20-year period, N-fertilization rate in this area has increased from 90 kg N/(ha·yr) during the first 10 years to 120 kg N/(ha·yr) during the following period. The higher amount of N-fertilizer used during the second 10-year period caused a distinct increase in simulated nitrate leaching, mainly when turnover of organic matter was assumed to be rapid (fig. 4). Observations showed a pattern similar to that simulated by the fast-turnover approach, while the simulation assuming a slow turnover of organic matter led to an obvious underestimation of nitrate leaching during the final years.

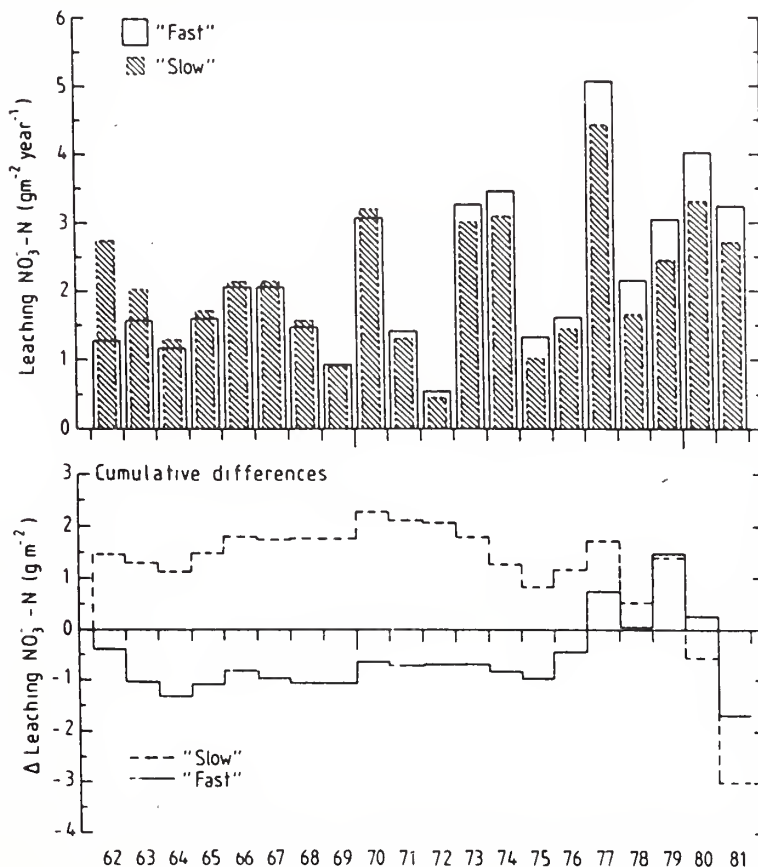


Figure 4.
Annual amounts of simulated leaching
with two different parameter sets
and cumulative differences between
simulated and measured leaching.

The increased N-fertilization resulted in higher crop yields and thus also in a larger crop-residue input in the model. In the fast-turnover approach this led to an increased net mineralization. However, the slow turnover of organic matter increased immobilization and therefore decreased net mineralization compared to the first 10-year period. In both simulations the model predicted that the additional N-fertilizer input was mainly taken up by the crop, and only a small fraction was lost directly from the system due to leaching.

Although there was a general lack of detailed information from the watershed, the results showed that both organic-N fractions in the soil contributed to the simulated change in leaching associated with increased N-fertilization. The question remains if a higher rate of net mineralization, following increased crop residue input, will occur within a couple of years or will require decades after incorporation of residues.

Perspectives

Since the model described here is representative of a whole group of simulation models dealing with nitrate leaching and nitrogen transformations in agricultural soils, comments and suggestions for model improvements are also applicable to many other nitrogen models.

Characteristic of most of these models, despite similarities in structure, is that they usually emphasize certain processes while treating others more superficially. To be suitable for management and regulation, models should be balanced. The use of a fixed potential uptake curve to control plant N-uptake is one example of a crude simplification in the model described here. No climatic factors, such as drought stress, are considered, which is a shortcoming when nitrate leaching during longer periods is simulated. Another example is the oversimplified treatment of denitrification, which is a common problem with models dealing with nitrogen transformations in agricultural soils. However, the simulated annual amounts of N denitrified in the Kjettslinge applications were similar to preliminary estimates, based on field measurements (Klemetsson 1986), which is satisfactory for a model intended for use in management. Further experimental studies are needed to make a critical test of the denitrification part of any model possible.

Some processes and parameters were identified, in the applications cited above, as being crucial for accurate simulation of nitrate leaching from agricultural soils. Assumptions concerning N-flows between organic-N pools were shown to play an important role in the watershed simulation, when leaching trends are investigated. It is still difficult, however, to predict how changes in agricultural practices in the model will affect soil organic matter and the flows between the organic pools. Another example is crop N-uptake and parameters associated with this process. Common both in decomposition/mineralization of nitrogen and plant N-uptake is the high magnitude of these N-flows. For example, simulated annual N-uptake by the grass ley at Kjettslinge was about 400 kg N/ha and simulated mineralization was about 200 kg N/ha. This is in contrast with simulated leaching (fig. 3) and denitrification, which averaged only 10 and 5 kg N/(ha·yr), respectively. Thus even small variations in plant N-uptake and/or N-mineralization can easily overshadow changes in mineral-N content and N-leaching. Consequently, it is very important to accurately simulate these large N-flows in order to get good estimates of nitrate leaching. This is especially important when dealing with management and regulation, for which accurate quantification is crucial.

Discrepancies between simulated and measured leaching in the Kjettslinge applications were mainly explained by uncertainties in hydrological flow paths rather than by uncertainties in biological processes. This suggests that it would be a substantial improvement to add a mechanism for water flow in macropores to the model, similar to that described by Jarvis and Leeds-Harrison (1987). However, their model does not, at present, include solutes. A bypass mechanism in structured soil is also considered in a model described by Addiscott (1977, see table 1) which includes solute transport; it is simple to use and suited for management purposes. This model, however, is not based on soil physical theory, which somewhat limits its general applicability.

An obvious advantage of the physically-based water and heat model described here is that it can be adapted to different sites by using available texture information (cf. Jansson et al. 1987). Moreover, driving variables are derived from standard meteorological variables. Both these factors make more widespread use possible.

Case Study 2: Leaching of Phosphate

Phosphate is considered the limiting nutrient as far as eutrophication of surface waters is concerned. Although agriculture is certainly not the only source of phosphate pollution, it is nevertheless a major one, perhaps the most important nonpoint source. The problem is most serious in those regions where a very intensive form of agriculture is practiced on soils with a limited capacity to hold phosphorus, e.g. in pig-breeding areas on light soils in The Netherlands, Belgium and West Germany. In some of these regions, disposal of large amounts of animal slurry on a relative small area has created a situation where the phosphorus sorption capacity of the soil is almost reached.

The Dutch government has enacted legislation that limits application of animal slurry on soils. Because additional future regulations will be based on studies done by Van der Zee and Van Riemsdijk (1986), we decided to use their work in our case study on phosphorus. The specific paper we will discuss deals with transport of phosphate on a column scale and in a field situation. The model considers non-calcareous sandy soils.

Structure of the Model

First transport in a single column is treated. In principle, here the basic transport equation 1 without the production/consumption term applies. Because of the nature of phosphate sorption by the soil, one can expect a relatively sharp front to develop, so it was considered justified to neglect dispersion and diffusion. The governing equation then is:

$$\rho \frac{\partial F}{\partial t} + \theta \frac{\partial c}{\partial t} = v \frac{\partial c}{\partial z} \quad [4]$$

where F is the sum of adsorbed and precipitated phosphate. The field is supposed to consist of an ensemble of such columns.

Sorption

Sorption is modeled as two processes: a short-term Langmuir-type adsorption (equilibrium reached in about one day) and a long-term diffusion-controlled precipitation (pseudo-equilibrium reached after several months). This description of phosphate behavior in soil is based on numerous earlier publications (Beek (1979), Lexmond et al.(1982), Van Riemsdijk and De Haan (1981), Van Riemsdijk and Van der Linden (1984)) dealing with the different aspects of the physico-chemical interaction between phosphate and the soil matrix.

Transport

Column scale. When slurry is applied to the soil surface the concentration there will be buffered at a particular value, c_0 , until all solid phosphate in the slurry has dissolved. Accordingly the boundary condition at the soil surface in the case of such a slurry application can be approximated by a Heaviside step function:

$$z = 0; \quad c = c_0 H(t^* - t), \quad [5]$$

where t^* is the period in which all solid phosphate is dissolved and the step function $H(x)$ is defined as: $H(x) = 0$ for $x < 0$, and $H(x) = 1$ for $x > 0$. Solving equation 4 then yields:

$$F = F(c_o)H \left\{ \frac{vt^*}{R} - z \right\}, \quad [6]$$

where $R = 1 + \rho F(c_o)/\theta c_o$. For a sequence of M applications of slurry the P-front can be approximated by:

$$F = F(c_o)H \left\{ \frac{M \sum t_i^*}{R} - z \right\} \quad [7]$$

$F(c_o)$ can be approximated by the sorption capacity, evaluated at the buffering concentration, $F_m(c_o)$. One calculates F_m from the content of amorphous aluminum and iron oxides in the soil, which can be assessed by extracting the soil with acid ammonium oxalate. With this extraction, almost all soil phosphate is also extracted.

Equation 7 can be rewritten as:

$$F = F_m H \left\{ \frac{P_{ox}}{F_m} - \zeta \right\} \quad [8]$$

where P_{ox} is the oxalate-extractable quantity of soil P. Because P_{ox} and F_m are depth-averaged quantities (averaged over a depth of L m), the ratio P_{ox}/F_m gives the degree of saturation of a column of length L , at the time of sampling. The dimensionless depth ζ is defined as :

$$\zeta = \int_0^z (Fe + Al)_{ox} dz / \int_0^L (Fe + Al)_{ox} dz \quad [9]$$

In equation 9, $(Fe + Al)_{ox}$ is the sum of the oxalate-extractable amounts of Fe and Al, which are generally a function of depth z . From equation 8 it follows that the dimensionless concentration of P in the solid phase is:

$$\Gamma = F/F_m = H \left\{ \frac{P_{ox}}{F_m} - \zeta \right\} \quad [10]$$

Results

Field scale. The field is assumed to consist of an ensemble of columns, each with its own P_{ox} and F_m , both of which are considered to be randomly distributed.

In a field experiment, on a sandy soil, the soil profile was sampled shortly after the harvest of the crop (corn) at 67 locations. In each of these samples P_{ox} and $(Fe + Al)_{ox}$ were determined. Both P_{ox} and $(Fe + Al)_{ox}$ were found to be normally distributed. With the computed statistics of P_{ox} and F_m the field-averaged profile may be calculated, assuming that P_{ox} and F_m are independent. This can be compared with the field-averaged experimental profile, as is done in figure 5. Experimental and computed profiles are in reasonably good agreement, although the former follows a somewhat steeper course.

Perspectives

The model is relatively simple and is reasonably accurate, when a particular situation is described. However, to use it for predictive purposes the spatial nature of the random variables should be known, e.g., the occurrence of a certain trend in the spatial variables and the correlation between variables. As yet this appears to limit a routine application of the model.

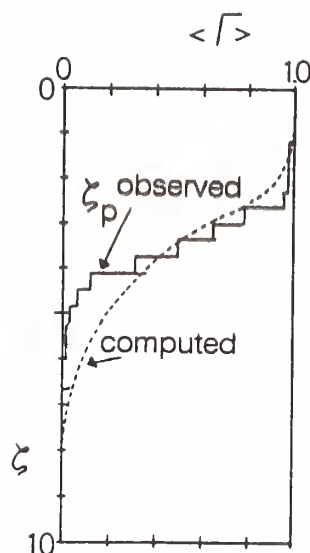


Figure 5.
Average dimensionless concentration of P in the solid phase $\langle \Gamma \rangle$ (see equation 10)
as a function of dimensionless depth ζ (equation 9).

Despite model limitations, the insights gained with the model have made it possible to formulate a protocol (Van Der Zee 1988) for phosphate-saturated soils. The protocol is a set of procedures for the details of soil sampling, soil sample treatment and laboratory analysis, and data evaluation, to which (in principle) each field is subjected in a region suspected of harboring many phosphate-saturated fields. It will be used to estimate the maximum permissible thickness of the phosphate-saturated topsoil, as a function of adsorption and fixation (precipitation) parameters and the depth of the groundwater table. As such it will be used to extend and supplement existing regulations.

Case Study 3: Leaching of Pesticides

Although simulation models for transport of pesticides have been designed for more than a decade in Europe (Leistra 1972), apparently they have not been used specifically for planning, management and regulation (Leistra and Boesten, pers. comm.). In The Netherlands, admission of new pesticides is, among other things, based on studies of Leistra (1975), Leistra and Dekkers (1976) on adsorption, decay, and transport of such substances. Boesten (1986), elaborating on Leistra's work, presented an extensive and detailed study on simulation models for the behavior of herbicides in soil. Although his model has not yet been used for management purposes, in our opinion it offers sufficient possibilities to do so. Therefore we selected the thesis of Boesten as a case study. In this thesis both instantaneous and time-dependent nonlinear sorption of the herbicide are taken into account, in addition to transformation and transport.

Structure of the Model

The numerical solution of equation 1 is obtained by a finite-difference approach. The 40-cm soil profile is divided (from top to bottom) into 10 0.05-m thick layers, 15 0.01-m thick, and 10 0.02-m thick. The calculations pertain to a non-cropped soil.

Sorption and Decay

From both short- and long-term batch experiments it was found that for the herbicides in question three classes of sorption sites had to be distinguished. The total bulk density of the herbicide in soil can thus be given as:

$$C = \theta c + X_1 + X_2 + X_3 \quad [11]$$

where θ = the volumetric water content, and
 X_i = the amount sorbed on sites of class i in mass per unit soil volume.

Sorption on sites of class 1 was found to proceed so fast that instantaneous equilibrium can be assumed, whereas sorption to, or desorption from, class 2 and 3 sites was found to proceed at finite rate:

$$X_1 = K_1 c^{(1/n)} \quad [12]$$

$$dX_2/dt = k_2 \{K_2 c^{(1/n)} - X_2\} \quad [13]$$

$$dX_3/dt = k_3 (K_3 c - X_3). \quad [14]$$

Equilibrium for class 1 and 2 sites is described by a Freundlich isotherm (with parameters K_1, K_2 and n), and for class 3 by a linear isotherm (with parameter K_3). Rate constants are given by k_2 and k_3 , the latter being one order smaller than the former (values are about 0.5 day^{-1} and 0.02 day^{-1} , respectively).

Decay of the herbicide was described according to first-order kinetics:

$$S = k_1 \theta c \quad [15]$$

Transport

Transport by water is an important component of total transport, so the model contains a routine by which flow of water is calculated. The flow of water is described by a "functional" model (Addiscott and Wagenet 1985), i.e., instead of calculating fluxes of water in a fundamental way a simpler approximation is used. This approximation is for downward flow (e.g., when rainfall exceeds evaporation) similar to the method proposed or used earlier by Terkelstou and Babcock (1971), Burns (1975), Van Keulen (1975), and Stroosnijder (1982). Precipitation in excess of evaporation fills the soil layers from top to bottom to water content at field capacity. The resulting flux to the next lower layer can thus be estimated.

Evaporation is estimated as 90% of the Penman evaporation as long as the cumulative potential evaporation is less than a soil specific value, β^2 . If cumulative potential evaporation (counting from the first day that evaporation exceeds rainfall) exceeds this value, actual cumulative evaporation is taken to be the product of β and the square root of the cumulative potential evaporation. From the cumulative actual evaporation, the actual evaporation rate (the flux of water leaving the soil surface) is calculated. A withdrawal function, giving the fraction of the surface flux withdrawn from a specific layer as a function of its depth below the soil surface, is employed to estimate the fluxes of water between neighboring layers. The water flow model has been validated with results from two years' field experiments. Figure 6 shows a comparison of calculated and measured water content for a particular year (1981), and demonstrates the good agreement between simulation and measurement.

In addition to transport by flow of water, transport by diffusion and dispersion are also considered (see equation 1). The diffusion coefficient D_{dif} for the herbicide was taken from the literature, whereas the dispersion coefficient D_{dis} was calculated as:

$$D_{\text{dis}} = |v| \ell \quad [16]$$

where ℓ is the dispersion length, which was estimated from field experiments with bromide as a tracer.

Results

The performance of the simulation model was tested with results of field experiments, where the values of the necessary parameters had been determined in independent batch and field

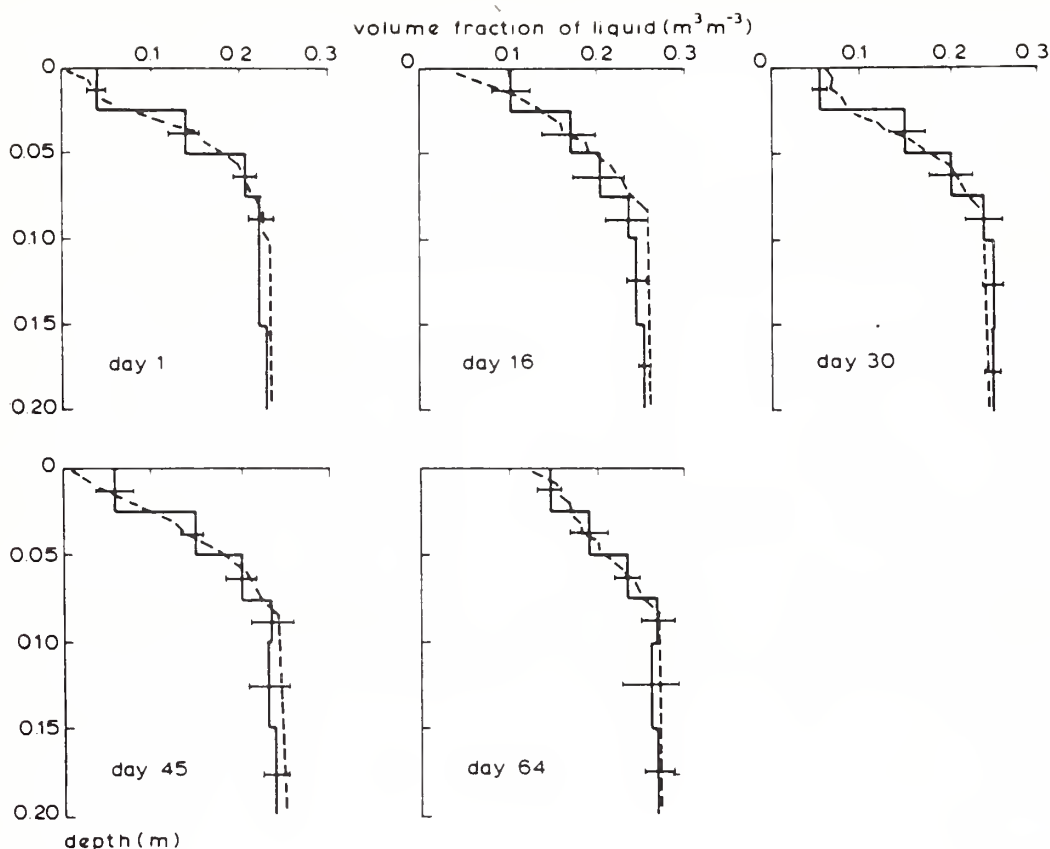


Figure 6.
Profiles of water content on 1981 sampling dates in a field experiment.
Vertical solid line segments are averages of 5 measured profiles; horizontal bars are standard deviations; and dashed lines are simulated profiles.

experiments. The soil simulated was a loamy sand, containing 1.8% organic matter, 3.6% CaCO_3 (pH 7.4 in 1 N KCl), and was fallow during the 64-day experimental period. Figure 7 compares measured and predicted soil profile concentrations of metribuzin at five times during the simulation period. The model results are in good agreement with the experimental results.

Perspectives

This model appears to be well balanced. It includes the processes relevant for the phenomenon studied. Although simplicity was an objective (e.g., the calculation of water flow), no process description was simplified for the sake of simplicity alone.

The model has been properly validated with independent experiments. The results of the validation, which appear to be quite good, therefore give a fair impression of the reliability of the model. The model thus seems applicable on other sites.

The model demands quite a few parameters: i.e., seven for the physico-chemical part, to which the number of parameters governing transport, also seven, has to be added. Some of these parameters (e.g., water content at field capacity or soil bulk density) are relatively easy to estimate or can be obtained by simple standard measuring routines. Others (the parameter β governing evaporation, or especially the parameters connected to sorption to class-3 sites) call for rather complicated or time-consuming experimental estimation methods.

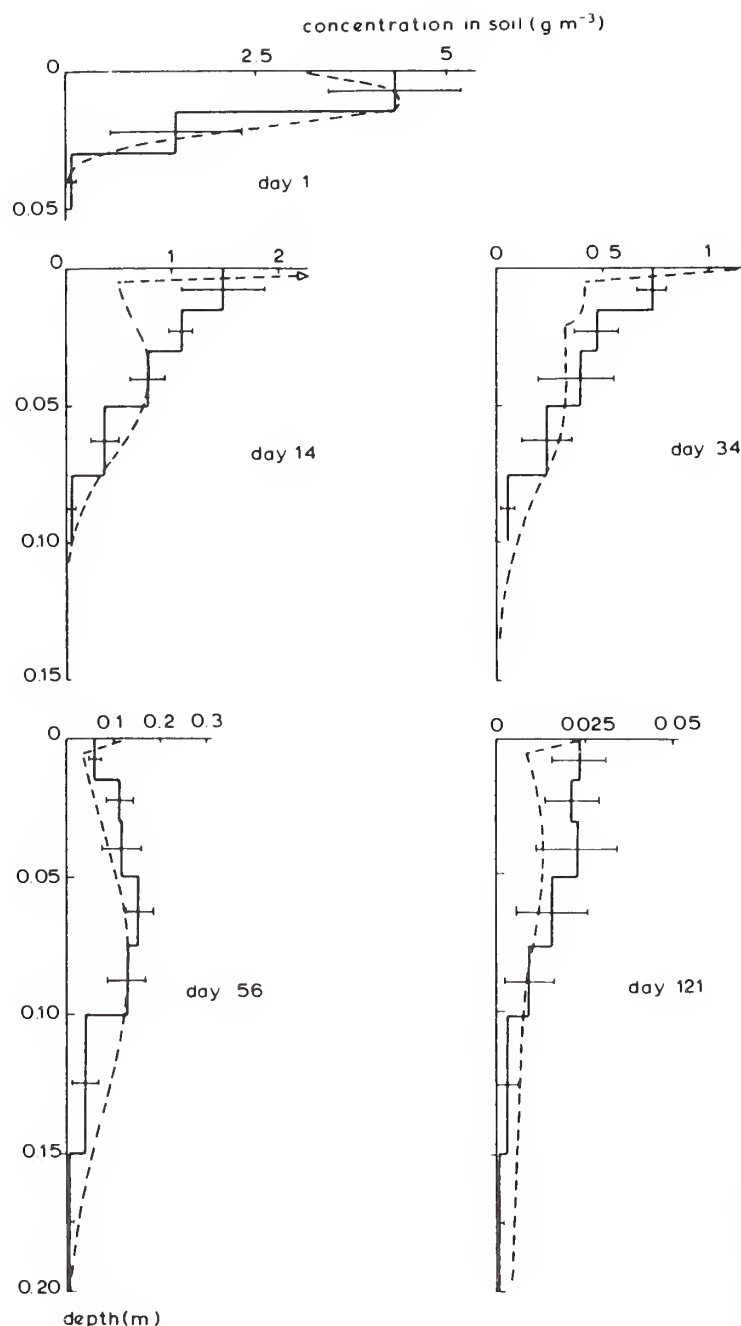


Figure 7.
Comparison of calculated and measured profiles of the herbicide metribuzin. Vertical solid line segments are averages of measured concentrations; horizontal bars are standard deviations; dashed lines are calculated.

An obvious extension of the model is to consider also the period in which the soil is cropped. Then also, among other things, uptake of herbicides and water by the plant should be included.

CONCLUDING REMARKS

The development of simulation models appears to be one of the routine methods used when problems of pollution and leaching are encountered. This practice has led to a plethora of models, which often at first sight, and indeed also after detailed inspection, are quite similar. One suspects that in many cases the real incentive for developing yet another model is not so much the application of computer modeling to an unexplored area, but is what Van Keulen et al. (1981) have called: the attitude that implies "anything you can do, I can do better", if not a basic coolness

to, or mistrust of, the complex models of others. On the other hand, there is some justification for a decision to develop a new model despite the large number and diversity of existing models, because the way in which underlying concepts are programmed in models is quite often difficult to understand for users other than the original developer. Furthermore, technical problems are often encountered when model implementation is attempted on different computer systems. Moreover, there is usually much understanding to be gained from developing one's own model, instead of copying someone else's.

In order to use models like those listed in table 1 for practical purposes, it is necessary to be able to estimate required parameter values from independent, standard measurements. An accurate and easily-available method to estimate parameter values would allow models to be applied to sites where detailed information on the temporal pattern of relevant processes is lacking. If parameter values can be accurately estimated, models that are more research-oriented may also be useful for analysis of practical questions concerning agricultural practices. If it is inevitable to use parameters that are site-specific and can only be obtained by complicated and time-consuming methods (e.g., determination of mineralization and denitrification rates), it is sometimes possible to correlate such parameters to easily-obtainable and/or time-independent system properties. Examples are the correlation between mineralization and soil texture (Van Veen et al. 1985, Richter et al. 1988), and between F_m and $(F_e + Al)_{ox}$ (Van der Zee and Van Riemsdijk, 1986; see case study 2).

As discussed earlier a prerequisite for a model to be attractive for users outside the designers' group (or indeed outside the scientific community) is the existence of appropriate documentation, in the form of a user's manual. Such a manual should discuss the relevant theory, explain how it is incorporated into the model, which language is used, what input is required, and of course the objectives for which the model was developed and is applicable. Also needed is a discussion of the model limitations, of the simplifications used, and it should be indicated when the model cannot be used. Moreover, it should contain information as to the determination or estimation of the parameters required; possibly it should suggest default parameter values which apply to an "average" situation. In Europe the existence of such user-friendly documentation for leaching models is the exception rather than the rule. Also for the models presented as case studies documentation, other than scientific papers, is lacking, though at least the protocol mentioned in the context of case study 2 offers the possibility of application of the model to practical situations.

Even well-tested and user-friendly models should be used with caution if employed by external users. Especially when used by non-modelers (e.g. planners and politicians), the danger exists of misinterpretation of results and of too much trust in model predictions. When a model is made available for practical use, the modeler should still be consulted for interpretation of the results because many far-fetched assumptions are used even in the best of models.

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REVIEW OF UNSATURATED ZONE LEACHING MODELS FROM A USER'S PERSPECTIVE

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ABSTRACT

A variety of models exist for estimating movement and degradation of agricultural chemicals in the unsaturated zone. General-use, mechanistic models include PESTAN, MOUSE, PRZM, CMLS, GLEAMS, LEACHMP, and RZWQM. PESTAN is a steady-state model while the other six are transient models with varying levels of sophistication. The most appropriate model to use depends on the application and the quality of available data. Unsaturated-zone model-development activities need to include establishment of data bases or estimation procedures for input parameters, development of appropriate assessment procedures, and establishment of linkages with saturated zone models.

INTRODUCTION

Public concern over residues of agricultural chemicals in groundwater is a relatively recent issue in the United States, originating in 1979 when pesticide residues were discovered in drinking-water wells in California and New York. As a result of these and more recent findings of agricultural chemicals in drinking water wells, a flurry of research programs has been instigated by regulatory, university, and industry scientists. This research has included the development of unsaturated-zone models for predicting movement and degradation of agricultural chemicals.

Models for predicting movement of agricultural chemicals originated in the mid and late 1970's, primarily in Europe. Examples include work in the Netherlands (Leistra et al. 1976, Frissel and Reiniger 1974) and Great Britain (Addiscott 1977, Walker and Barnes 1981, Nicholls et al. 1982). Since 1979, model development research conducted in the United States has largely been performed or funded by federal agencies such as the EPA and USDA, although several models have been independently developed by university scientists.

This paper will review seven models (listed in table 1) developed in the United States for modeling movement and degradation of agricultural chemicals in the unsaturated zone. These models were selected considering three factors. First, these models are applicable to non-point agricultural sources (that is, for applications to fields rather than sources resulting from spills or landfills). Second, these models directly simulate the movement of agricultural chemical residues in the unsaturated zone based on physical processes (the models are mechanistic rather than empirical-although each model has some empirical elements-and predict actual movement for a specific set of conditions). Third, these models are available for general use (not just research models developed for a specific application). The scope of this paper was limited to those models which include the ability to simulate movement of pesticides and plant growth regulators. Models developed specifically for nutrients were not included, although much of the discussion in this paper is applicable to such models (nutrient models are discussed in three other papers from this symposium: Wagenet et al. 1989, Vachaud et al. 1989, and De Willigen et al. 1989).

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Table 1.
List of U.S. Mechanistic Models.

MODEL	DEVELOPER	MODEL TYPE	USER MANUAL	COMPUTATIONAL REQUIREMENTS	FREQUENCY OF USE
PESTAN	U.S. EPA	steady-state	no	minimal	widespread use until about 1985; currently is rarely used
MOUSE ¹	Cornell U.	transient	yes	low	low to moderate
PRZM	U.S. EPA	transient	yes	moderate	most widely used model
CMLS ²	U. of FL	transient	yes	moderate	moderate
GLEAMS ³	USDA	transient	yes	moderate	moderate
LEACHMP	Cornell U.	transient	yes	high	moderate
RZWQM ⁴	USDA	transient	yes	high	under development

¹Developed primarily as an educational tool with graphics.

²Model focuses on the position of the solute peak.

³Extension of the CREAMS model; currently applicable only to the root zone.

⁴Model and documentation currently being developed.

DISCUSSION OF SPECIFIC MODELS

This section presents specific comments about each of the seven reviewed models. The models are arranged in approximate chronological order of development.

PESTAN

Developed by the United States Environmental Protection Agency, this model became available in 1980 and is the earliest model of the seven reviewed in this paper. It uses a steady-state analytical solution to the convection-dispersive solute transport equation obtained by assuming one-dimensional constant flow in a homogeneous soil profile with constant hydraulic properties, sorption, and degradation parameters (Enfield et al. 1982). The lack of a users' manual poses little problem due to the simplicity of the model. Very little input data is required, although one parameter, net recharge velocity, may be difficult to estimate (for model comparison simulations, net recharge velocity is often obtained from the water balance portion a more complex model such as PRZM). Although the model assumes constant soil and chemical properties, changes in adsorption or degradation rates with depth may be approximated by superimposing simulations made under various conditions. One mistake often made by users of this model concerns the appropriate degradation rate. Unlike the other models discussed in this paper, PESTAN uses a solid-phase degradation rate, which is usually a factor of 3 to 5 lower than the overall degradation rate measured in most field experiments: therefore, when the overall degradation rate is used in PESTAN, the predicted degradation is a factor of 3 to 5 too fast. This model was widely used by EPA and industry scientists before the introduction of more comprehensive models such as PRZM, but today its original one-dimensional form is rarely used.

MOUSE

Developed at Cornell University, this model solves the transient convective-dispersive equation for solute transport using a simplified water balance (Steenhuis et al. 1987). Because the principal goal of the model was for user education rather than actual predictions, the solution is not as rigorous as in the other transient models. Also, a simplified saturated-zone component is included. The one-dimensional soil model assumes two layers, root zone and subsoil, with fixed values of soil and sorption parameters within a layer. However, the degradation rate can vary within a layer. Daily weather data can be generated by an internal routine. The model was written for an IBM PC and has quite good graphical routines for displaying water balances and chemical movement.

PRZM

Developed by the United States Environmental Protection Agency, this one-dimensional model numerically solves the transient, convective-dispersive transport equation using a simplified water balance (Carsel et al. 1984a). The users' manual for this model (Carsel et al. 1984b) does a good job of documenting this code and explaining how required model parameters can be obtained or estimated. PRZM also includes optional estimation routines for some model parameters. The model is flexible enough to allow simulation parameters such as soil properties and chemical degradation rates to vary with depth. However, a program to prepare input files is quite machine-specific and is not often used. Although the model requires daily weather data, a weather tape is available providing this information for at least 25 years at locations throughout the United States. Procedures for estimating soil parameters from information in the SIRS data base (Goran 1983, Thompson et al. 1987) are also available. The program can be easily modified to allow such changes as varying parameters with time or using kinetics other than first order. The availability of input parameters, the support provided by EPA to model users, and the use of PRZM by EPA in several regulatory assessments has contributed to considerable use of this model, especially by industry scientists. A new version of this model is being developed (RUSTIC) which will allow simultaneous prediction of both original compounds and metabolites, use the method of characteristics to improve estimation of dispersion in the soil profile, and include routines for estimating soil volatilization losses. RUSTIC will also include linkages with a vadose zone model based on Richards' equation and a saturated zone model.

CMLS

This one-dimensional model (Nofziger and Hornsby 1986) is a refined version of an earlier model PISTON (developed at the University of Florida by Rao et al. 1977). CMLS, written for an IBM PC, calculates the movement of a solute front using a simplified water balance. Although the model does not consider dispersion, retardation of solute relative to the movement of water is considered. Soil properties and degradation rates may be varied with depth. The model requires daily rainfall data as input.

GLEAMS

This model (Leonard et al. 1987) is an extension of the CREAMS runoff, erosion, and chemistry model developed by the United States Department of Agriculture (Knisel 1980). Currently GLEAMS is recommended for application only to the root zone. It solves the one-dimensional transient convective-dispersive equation for solute transport using a simplified water balance. Daily weather data is required but may be generated by an internal routine. Soil properties and degradation rates may vary with depth. The model can also calculate the transformation and movement of nutrients.

LEACHMP

Developed at Cornell University, this model is the only generally available one-dimensional unsaturated zone model which solves the water balance using Richards' equation (Wagenet and Hutson 1986). This additional complexity introduces an iterative calculation procedure which must converge at each time step. Under some circumstances, problems with convergence have been reported due to the non-linearity of the surface boundary condition. Computer time requirements are substantially greater for LEACHMP than for models using a simplified water balance. If the appropriate rate constants are supplied, LEACHMP can simultaneously predict concentrations of both original compounds and metabolites.

RZWQM

This model is currently being developed by the United States Department of Agriculture (Hebson and DeCoursey 1987). During the development process, a large number of regulatory, academic, and industry scientists were invited to make suggestions about the various algorithms to be used and how the model should be structured. Since all components of the model will be designed to incorporate the most rigorous estimation techniques, computer time requirements are likely to be quite high. A data base of chemical and nutrient properties will be included. The model is scheduled for release in 1989.

GENERAL DISCUSSION

Comparison of Models

As discussed in the previous section, there are many differences among the seven models. Two of the most fundamental differences are the methods used for calculating the water balance and for estimating dispersion.

The method of calculating the water balance is the primary difference between the seven models. Since PESTAN is a steady-state model assuming a constant recharge, it cannot accurately model areas with large variations in seasonal rainfall. However, by appropriate scaling of time and rainfall, this steady-state model can be used to approximate a transient situation, especially if the degradation rate does not change significantly with depth. Depending on rainfall patterns and the assumptions used in calculating net water recharge velocity, PESTAN predictions of solute movement may vary significantly from those predicted by the other models. Little difference in predicted solute movement would be expected between MOUSE, PRZM, CMLS, and GLEAMS since essentially the same simplified water balance (no movement until field capacity is exceeded, then instantaneous movement) is used in each of these models. Also, no upward movement of water in the soil profile (and therefore no upward solute movement) in response to evaporation losses at the soil surface is considered in the transient models with the simplified water balance. These assumptions sometimes result in these models overpredicting solute movement compared to field measurements (Jones et al. 1986). Because LEACHMP calculates the rate of water movement using the Richards' equation and accounts for upward movement of water, water movement and hence solute movement is slower than predicted by the models using the simplified water balance, especially in heavier soils. However, recent comparisons (Hornsby et al. 1988) have indicated that in sandy soils where the rate of water movement is relatively fast, the differences between the predictions of LEACHMP and the other transient models are not significant.

The transient models also differ in the method for calculating solute dispersion. The movement of the solute peak is calculated in CMLS and MOUSE, while in the others numerical techniques are used to calculate the movement in each soil layer assuming some value of dispersivity. When solute dispersion is calculated using finite difference or finite element procedures, numerical

dispersion may affect the calculated dispersion of a solute (finite difference techniques are more prone to numerical dispersion than finite element techniques). Thus the predicted solute dispersion (and therefore the concentration profiles) may be dependent on the depth increment. In MOUSE, the dispersion around the solute peak is calculated using the appropriately-scaled error function (similar to the procedure used in PESTAN). In CMLS, no dispersion around the solute peak is considered and therefore soil concentrations are not calculated by the model. However, this is not a serious deficiency compared to other models since calculated concentration profiles from any of these models usually do not adequately match measured profiles. Instead, the preferred way of reporting results is in mass or percent of applied material moving past a specified soil depth because such values are much less sensitive to the amount of dispersion and the shape of the concentration profile (for multi-year or Monte-Carlo simulations, the uncertainty of these values for mass flow can be expressed using a cumulative probability distribution). Also, it may be misleading to report concentration profiles since even in a relatively homogeneous field, concentrations of agricultural chemicals at a specific depth and time are likely to vary by at least two orders of magnitude.

Model Assumptions

Potential sources of error in mechanistic model predictions include the theory and assumptions that comprise a model, the numerical solution of model equations, and selection of input parameters. The user controls these errors by the choice of an appropriate model for the specified application and by correct specification of input parameters. Therefore, it is important for a model user to be aware of the assumptions inherent in a model. Then, when considering the use of a model for a certain application, the appropriateness of these assumptions should be examined. The validity of the values of each of the input parameters should also be considered. The appropriateness of extracting parameters from the work conducted at other locations or with other compounds should be reviewed.

Unfortunately, the above advice may conflict with the desire for a model to be "user friendly." Users typically want to minimize time spent reading manuals, and desire that a model provide default values for information that is not known or is difficult to obtain. Increasing the number of default values that are used in simulations may potentially increase the chance of erroneous simulation results. Since specific site information is often difficult to obtain, modelers are tempted to use information supplied by someone else for another location. In general, the ability to correctly simulate unsaturated zone movement is more dependent on the skill of the user to properly choose input parameters than the accuracy of the model (usually the simpler the model, the more subjectivity and professional judgement required to choose the model parameters). When model predictions are incorrect due to inappropriate input parameters, increasing the sophistication of model theory will not necessarily result in improved predictions.

Several assumptions are common to most of the models discussed in this paper. All assume first order kinetics for the degradation rate either for an overall rate of disappearance or for each reaction step. Degradation rates at a specified depth usually cannot be changed with time (for example, due to changes in soil temperature). Sorption is usually considered to be described by a linear isotherm with no difference between sorption and desorption. The models assume that concentrations in the liquid and solid phases are always in equilibrium. The appropriateness of these assumptions should be considered for each application. In some cases, the model can be modified by relatively minor changes in the code to eliminate a particular assumption (for example, changes in kinetics or sorption isotherms could be made quite easily if the data were available).

One of the most important factors determining movement of agricultural chemicals is the amount of water moving below the root zone. In all the models, water movement below the root zone (often referred to as the amount of recharge water), is calculated as the amount of rainfall and

irrigation minus the sum of evapotranspiration, runoff, and changes in water storage (usually the last term is an insignificant proportion of the overall water balance for simulations being conducted for times greater than several months). In many cases, the sum of rainfall and irrigation and the sum of evapotranspiration and runoff are relatively large compared to the amount of water moving below the root zone. Therefore the accuracy of the water recharge term is quite sensitive to the accuracy of the other terms.

Values for runoff and evapotranspiration losses are usually not measured directly and must be estimated. Some of the models do not consider runoff losses of water or agricultural chemicals, while models calculating runoff (PRZM and GLEAMS) use the Soil Conservation Service curve number approach. The curve number approach yields only field-average runoff values that vary only as a function of initial soil moisture and does not consider the effect of rainstorm intensity. In sand or loamy sand soils, where potential for downward movement is the highest, precise estimation of runoff is usually not needed since runoff (and chemical losses in runoff water) are typically quite small. However, in clay soils, a significant fraction of a rainfall event may move laterally off the field rather than moving downward through the soil profile.

One difficult step in most simulations is to obtain accurate potential evapotranspiration data. Often potential evapotranspiration is estimated from average daily temperature data or from pan evaporation data using an appropriate correction factor (pan factor and/or crop coefficient). Inaccuracies can result using either of the two procedures so the resulting evapotranspiration losses calculated during a model simulation should always be checked for reasonableness. The predicted solute movement has been substantially altered in several PRZM simulations depending on whether the potential evaporation was estimated using average temperature data or pan evaporation data. Often the estimation routine based on average temperature data has appeared to underestimate evapotranspiration and thus overestimate chemical movement compared to measured field results. However, the crop coefficient approach may also produce inaccurate estimates, especially at times when the crop cover is small and the amount of bare soil is large (Hanks 1985).

The models described in this paper are not designed to simulate movement of agricultural chemicals in irrigated fields, but the models can be used to provide estimates under certain conditions. Usually this is accomplished by adjusting the amount of rainfall on days when irrigation is applied (when agricultural chemicals are present on plant foliage in flood or furrow irrigated fields, this approach would not be valid due to overestimation of residue washoff). None of the models can be used in situations where irrigation is applied by raising the water table underneath a field and water is supplied by upward movement of water to the root zone. Also none of the models can be used to simulate movement in or below areas which are temporarily saturated (perched water tables) where significant lateral movement of water may occur. In fields where irrigation water is not applied evenly (such as with furrow or flood irrigation), the location of the agricultural chemical application relative to the location of irrigation furrows influences chemical movement. Therefore, model simulations may either overpredict or underpredict movement of agricultural chemicals in fields where irrigation is applied unevenly (Jones et al. 1986). Even when irrigation water is applied uniformly using some form of sprinkler system, model predictions may be in error. For example, for those models which consider runoff, excessive values of runoff may be predicted (thus underpredicting downward movement of water). One approach to reducing runoff losses from irrigation is to spread the amount of irrigation over more than one day in the simulation.

Another assumption made by all of the models is that macropore flow is not significant. Since macropores exist in finer-textured soils (while concern with groundwater residues is usually limited to coarser-textured soils), this assumption is not usually of concern. Ignoring macropore flow may result in either underestimating or overestimating movement of agricultural chemicals depending on their location. If chemical residues are located on foliage or the soil surface, water flowing

through macropores located at the soil surface may contain residues and the models will tend to underestimate movement. However, if residues are located in the soil (for example as a result of application methods which include soil incorporation), then water moving through the macropores do not come into contact with the residues and the models will tend to overestimate movement of agricultural chemical residues. In general, macropore flow has the potential to cause relatively low levels of agricultural chemicals to occur deeper (or faster) than the models predict, although data with aldicarb (Jones et al. 1986) indicate that macropores may have relatively small impact on the movement of relatively mobile agricultural chemicals in the unsaturated zone.

Model Selection

The appropriate model to use depends very much on the specific application. For example, if there is a need for an individual to become better acquainted with the general effects of various variables, then MOUSE is probably the model of choice because it is easy to use and has good graphical displays. If the application is to estimate whether a chemical is likely to move below the root zone in a specific location, then the use of PRZM, GLEAMS, CMLS, or MOUSE would be appropriate. If a more rigorous estimate is desired, then LEACHMP, PRZM, or GLEAMS probably should be used. PRZM, CMLS, MOUSE, or LEACHMP can be used for predictions of movement and degradation in subsoils below the root zone. Although more data and effort are required to produce simulations with LEACHMP, the use of this model is quite appropriate for comparing predicted versus observed movement in detailed field research studies.

All of the transient models give about the same results in light soils. However, in heavier soils the predicted movement of LEACHMP will be significantly less than that predicted by PRZM, GLEAMS, MOUSE, or CMLS (in general, movement of agricultural chemicals in heavier soils is of little consequence for groundwater residue concerns, since most instances of agricultural chemical movement through agricultural fields occur in lighter soils). LEACHMP will probably provide the most accurate predictions of chemical movement in heavy soils. The other transient models can be used to estimate an upper bound on chemical movement as long as the model user realizes that actual movement may be considerably less than predicted. The increased data and computational requirements of LEACHMP probably preclude its use for assessment techniques involving many individual simulations. However, if such assessments indicate a potential concern in areas with heavy soils, selected simulations should be performed with LEACHMP.

The quality of user support available for specific models may significantly influence model selection. The availability of information on model parameters in the format required by a model, the ability for users to obtain assistance for problems, and comprehensive user manuals facilitate model use. Also, a support group can collect errors that are discovered by model users and better understand user applications so the model can be improved through corrections and revisions.

Data Bases

The transient models require significant amounts of input data, including weather data, soil properties, chemical properties, crop parameters, and chemical application information. As mentioned earlier, the PRZM manual describes techniques for estimating parameters used in this and other transient models.

Although weather records are readily available from the National Oceanic and Atmospheric Administration, the daily weather data requirements of the models are often the greatest deterrent to performing model simulations, especially the 20 year simulations needed to assess climatic variability (weather data is available in monthly pamphlets or can be ordered on magnetic tape, but the latter option can be quite expensive). As discussed earlier, the EPA has made available a weather tape providing weather data required by PRZM for locations throughout the United States. With minor adaptations, this information can be used to provide weather data for other

models. Due to the limited number of locations within a state, this tape is useful primarily for general assessments. Weather data for comparing field research results with model predictions will usually have to be entered manually from NOAA publications or site measurement logs.

Two of the transient models, GLEAMS and MOUSE, try to reduce weather data input requirements by including an option for internally generating weather data. Although long weather records are needed to appropriately estimate the parameters required by the weather simulation routine (when such parameters are not already available), the use of a weather simulation routine greatly reduces the effort required in data input. Of course, for comparing predicted versus observed results, actual weather data would still have to be entered. The use of weather generators is appropriate when models are used for training purposes or for drawing general conclusions; however the use of actual weather records is preferred when making more comprehensive assessments (since the weather data generator is an approximation of the actual records, the use of actual records helps eliminate any biases that might result from the generation procedure).

The required soil parameters for the transient models that use the simplified water balance can be estimated from the information collected by the Soil Conservation Service and published in county soil surveys. The information is also available in the SIRS data base (Goran 1983, Thompson et al. 1987). However, the organization of the data base makes finding the distribution of specific soils within a state quite cumbersome. To address this problem, the EPA has recently completed preparing a subset of SIRS including only data related to the location and use of agricultural soils and their properties pertinent to unsaturated-zone movement. This new data base, DBAPE, will allow model users to identify the amounts and locations of soils fitting specified criteria and to obtain model parameters for these soils.

Typical Applications

Unsaturated-zone leaching models can be used in a variety of applications. One common use is model validation, in which simulations are performed and the results compared with field measurements (these applications may be directed toward testing theory as well as the model). Most of the references provided for the models discussed in this paper provide examples of this type of model application. Another use of such models is to assess the potential for movement of agricultural chemicals below the root zone or into groundwater. Although this is perhaps the most common use of models, relatively few examples of this type of application have been published (examples include Carsel et al. 1988ab, and Jones 1986). Also, models have been used in the development of best management practices such as optimization of application timing (Jones et al. 1983) or developing restrictions on applications of agricultural chemicals near shallow potable wells (Jones et al. 1987).

Assessment Procedures

Model application procedures are as important as the models themselves in drawing appropriate conclusions about mobility of agricultural chemicals. Assessment procedures need to account for year-to-year variations in climatic parameters (especially rainfall and evapotranspiration) and for significant changes in soil parameters even with sub-county units. Effects of variations in weather conditions on chemical movement have been illustrated by performing simulations using 15- to 30-year periods of weather data and expressing the results in a cumulative frequency distribution or a cumulative probability distribution (Carsel et al. 1984b). The effect of soil variability has been illustrated using Monte-Carlo techniques (Carsel et al. 1988ab) and performing simulations for all soils on which a specific crop is grown in a region (Jones 1986).

Linkage to Saturated Zone Models

If the appropriate model simulations indicate no movement of residues to the water table, then the assessment is complete. However, if the model predicts residues will enter groundwater, additional information is needed about the movement and magnitude of these residues in groundwater. Such information can be obtained by coupling the unsaturated zone model to a saturated zone model. This coupling is usually made by considering the residue movement predicted by the unsaturated zone model as input for the saturated zone model. Examples of such linkages in the literature include Jones et al. (1987), Dean and Atwood (1985), and Carsel et al. (1988a). As with unsaturated zone models, the choice of models will depend on the application. Cases involving site-specific comparisons of predicted and observed measurements will require more rigorous models than more general simulations. As illustrated by Carsel et al. (1988a), the use of even a simple saturated zone model can often be adequate.

RECOMMENDATIONS

The sophistication appropriate to modeling movement of agricultural chemicals in the unsaturated zone depends on the specific application and the quality of the available input data (for example, it is inappropriate to model movement with the precision of the Richards' equation if the soil type is not known). Therefore, models of various complexity need to be available to provide adequate levels of sophistication. Of course as model sophistication increases, the input data and the computational time requirements increase. The need for various levels of complexity can be met by the development of different models or by the inclusion of several different optional calculation routines within the framework of one model.

Model documentation should include a section that clearly lists the assumptions and limitations of the model. This section should include discussion on the effect of each assumption, the types of applications for which the model is best suited, and types of applications where the use of other existing models would be more appropriate.

Model development should include the establishment of data bases to supply required input parameters or the development of estimation techniques for obtaining such input from existing data bases. Such information is needed to generalize specific field or laboratory measurements to the wide range of climatic conditions and soils needed in performing appropriate assessments of leaching potential.

Unsaturated zone models should have linkages with saturated zone models to evaluate the magnitude and movement of agricultural chemical residues reaching the water table.

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DISCUSSION OF PAPERS PRESENTED IN TECHNICAL SESSION 1, PARTS 1 AND 2: LEACHING MODELS FROM THE MODELER'S AND USER'S PERSPECTIVE

Lynn M. Dudley¹, Presiding
Howard M. Deer², Recorder

PAPERS DISCUSSED

Predictive Approaches for Leaching in the Unsaturated Zone by R.J. Wagenet, M.J. Shaffer and R.E. Green

Solute Transport in the Vadose Zone: A Review of Models by G. Vachaud, M. Vauclin and T.M. Addiscott

Leaching Models of the Unsaturated Zone: Their Potential Use for Management and Planning by P. De Willigen, L. Bergström and R.G. Gerritse

Review of Unsaturated Zone Leaching Models from a User's Perspective by R.L. Jones and R.J. Hanks

SUMMARY

Modelers and model users expressed many of the same concerns regarding the state-of-the-art in leaching models. In both question and answer sessions the greatest portion of the discussion was on the following topics: model verification and validation, model application, model limitations and assumptions, and accounting for temporal and spacial variability. The topic of verification took the largest proportion for the time allowed for discussion in both sessions. The proper focus on and application of models were also topics of considerable discussion in both sessions. The two groups (modelers and users) differed in the time spent in discussion of other topics. Model users were very concerned about being able to understand the assumptions written into a given model, while there was only a brief discussion of model assumptions in the modelers' session. Conversely, a significant portion of the modelers' discussion time was devoted to uncertainty and variability, while the discussion of these topics in the users' session was limited. Variability and uncertainty were peripheral topics in the users' discussion of application of deterministic models to predicting solute loading of groundwater. Discussion of variability and uncertainty in the modelers' session included applicability of theory to field problems, determination of parameter probability distributions and methods for field experiments. With the exception of some specific comments on stochastic models, most of the discussion was directed toward deterministic models. Unless otherwise stated, it should be assumed that deterministic modeling was the subject of discussion. (No effort was made to identify the names of contributors).

SPECIFIC QUESTIONS AND COMMENTS

Question: What constitutes a model validation?

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Discussion: Considerable confusion exists regarding the difference between validation and calibration but it is agreed that both cannot be accomplished on the same data set. While this concept might appear straightforward, a proper validation experiment is a complicated proposition. It is generally agreed that field experiments which range in soils and climates and are long-term would provide the best data set for validation. However, field studies that are sufficiently intensive for model validation and are long-term are expensive and rare. Further, a proper field experiment may not be possible using existing methods. In order to validate a model, the data for parameter estimation, for driving the model, and for model validation should be collected on a compatible scale. This is, in fact, never the case in a field experiment. The data are commonly taken from samples which vary in scale: e.g., an auger, a ceramic cup, and shovel. Our field methods have not kept pace with the demands for testing our theories, and research resources should be devoted to this area.

Comment: Those who model often do not have the resources to conduct the field experiments.

Discussion: Field experiments are so costly that parameter collection and validation often are attempted employing the same data set. This common condition obviously does not constitute validation. Data bases for model development might be located through the CRIS systems in the U.S. and DG12 in Europe.

Comment: There is a need for cooperation among the users and modelers to facilitate validation.

Discussion: Validation could be accomplished by making a model available for application to a variety of field problems. While the model may never be validated, in the strict sense, by such a process, the confidence level in the model's predictive capabilities are increased.

Comment: Users are concerned with being able to identify models that have been validated or extensively tested.

Discussion: None of the available leaching models have been validated. The modeler does not validate because the comparison between model predictions and experiment becomes a process of model revision and refinement. The user does not validate because model parameters must be collected from the same data set for which predictions are made, or model predictions are used to compare resource management strategies and never compared to data. The model user should compare model predictions to field collected data until the user is satisfied that model predictions are sufficiently reliable for a given application. Such a process is not a validation, but involves gaining a level of confidence in model predictive capabilities. In the end, it is the responsibility of the model user to insure that model prediction makes physical sense. A multi-disciplinary approach may be a way of increasing confidence in model predictions.

Comment: Closely related to model validation is model application, in that models are created for and tested on specific types of problems.

Discussion: There are three principle concerns regarding model application: what is our objective in creating models?, how does one select a model?, how can we insure proper parameterization?, and how can we insure proper interpretation of model predictions?

Note:

The discussion in the session on the modeler's perspective included some comment on the objective of modeling. It was generally agreed that the primary objective of deterministic modeling is to summarize the state of knowledge in a quantitative way. The model becomes a tool to test our understanding of system behavior; the best use of a model is as an investigative tool. For the user, this translates to the maxim that models do not substitute for field experiments.

They can be effectively used to focus field experiments reducing costs and maximizing information.

Comment: Because models are often created with a bias of application to a specific problem, they contain many assumptions and simplifications that may not be appropriate for use in a different context. The problem to which the model is applied determines the requirements with respect to input parameters and model output.

Discussion: Model users are obviously confused by the number of models available and desire help from the modelers in selecting models. User-friendly codes, better user manuals and direct communication between modelers and model users may be ways to make it easier for the user to select a model most appropriate for their problem. Some of the modelers resist making codes user-friendly and providing better documentation. The perceived danger is that easily-used models are easily-abused models. The user should have a complete understanding of a model before applying it.

Question: What about model parameterization?

Discussion: According to modelers, one of the most significant sources of error in model application is inappropriate selection of model parameters by the user. However, the user is the only one who can be responsible for estimation of parameters, and they are encouraged to seek assistance from those experienced in modeling. From the users' perspective, those experiencing frustration over their attempts to apply existing models are reminded by the experienced users that the judgement which is only gained through experience, is often required in the selection of model parameters.

Comment: A model is misapplied if predictions are used in a more restrictive sense than the model is designed to furnish.

Discussion: There is a great deal of concern over the use of models by regulatory groups. Models do have a function in a regulatory environment as a means of identifying potential for contamination and comparison of compound behaviors. There is also potential for misuse when model predictions are taken as fact rather than demonstration of theory. A great deal of interest has been expressed by those identifying themselves with regulatory agencies in linking deterministic models of solute leaching with groundwater models. Those focusing on the use of such a model as a way of predicting solute loading in and migration in groundwater think this would be a pointless and dangerous exercise without accounting for spatial and temporal variability in the model parameters. Others focused on the capability of such a model for demonstration of solute behavior under specific conditions and for identification of solutes or management practices which might impact groundwater quality. From this perspective, model linkage was judged to be a valid undertaking.

Question: What should be the role of the modeler in model documentation?

Discussion: It is the wish of the users to have explicit statements regarding limitation accompany the model. However, modelers resist this idea; they feel that it is the users' responsibility to determine the model limitations and assumptions through careful examination of the code. Modelers may not be aware of all the assumptions and limitations of their model.

Comment: Typically, models are unbalanced in their treatment of the web of processes which influence solute leaching. Models generally have a more rigorous treatment of processes with which the modeler is most familiar. Models developed by soil physicists, for example, may include one or more two-dimensional finite-difference solutions to Richards' equation and the

convective-dispersive equation and only a linear adsorption coefficient to describe a number of chemical processes or compounds.

Discussion: It is generally agreed that progress will be made by those who can form multidisciplinary teams able to combine existing knowledge into more balanced models. The examples provided were more sophisticated treatment of chemical reactions, microbial processes, and plant water relations and nutrient uptake.

Note:

Models users discussion did not specifically include mention of stochastic models. The reason for this was stated in the modelers session as an acknowledgment of the paradox that to use a stochastic model one must know the probability distributions of parameters and in determining the probability distribution, need for model predictions may be eliminated. Extensive investigation required for the determination of probability determinations often is prohibited by cost. Most of the models presented were deterministic and could be used to compute probability distributions only by multiple executions. Multiple executions use probability distributions of model parameters or Monte-Carlo techniques.

Comment: The commonly-used models are not structured to deal directly with uncertainty and variability.

Discussion: Uncertainty and variability are topics of considerable interest to modelers. These areas are topics of much modeling research. Clearly, regulatory and resource management users desire predictive models. This requires that variability of model parameters and uncertainty of model estimates be addressed. Addressing these problems necessitates consideration of other problems, those of scale and appropriateness of our current models.

Note:

A number of suggestions and specific problems were forwarded. There were two central themes in the discussion: model calibration and validation appropriate to the scale of prediction and theoretical soundness of Darcy's law and the convective-dispersive equation at the field scale. Ideally, model parameters should be estimated from samples taken such that they represent the scale for prediction and data for model validation. It was suggested that only through an experiment of this nature can the validity of our current theories be tested. However, the representative scale of sampling techniques has not been determined. The question that follows from this argument is have our theories been properly tested? On the other hand, macropore flow may not obey Darcy's law and the behavior of a solute traveling through a macropore may not conform to the convective-dispersive equation. It was pointed out that some problems permit simplification of soil models avoiding use of the theories in question. The example was offered of overriding effects of variability in the surface boundary which may eliminate the need to consider soil variability. Capacity models can be used in simplification. These models use parameters which are less variable and can be collected at a larger scale; however, they are not well adapted to the prediction of fluxes.

Comment: Rigorous treatment of complex surface geometry and treatment of temporal changes in macroporosity and hydraulic conductivity are research areas for improving models.

Discussion: Finite difference models are not readily adapted to complex surface geometries. There are a few finite element models that can deal with uneven surface boundaries and could be applied to problems such as flow to a furrow top. Temporal changes in the hydraulic conductivity of a tilled soil over the first few rainfall events are greater than spatial variability. This temporal variation might be accounted for by a time-dependent characteristic curve.

AGRICULTURAL NONPOINT-SOURCE RUNOFF AND SEDIMENT YIELD WATER QUALITY (NPSWQ) MODELS: MODELER'S PERSPECTIVE

Calvin W. Rose¹, W. Trevor Dickinson², Hossein Ghadiri¹ and Sven E. Jorgensen³

ABSTRACT

This paper reviews models developed to represent the surface hydrologic processes which affect the delivery to streams by water and water-borne sediment and other nonpoint-source pollutants. The review considers what has been achieved by the current development of modeling activity, and gives some specific conclusions from a modeler's perspective. Current dilemmas are defined and issues and directions for research which should be considered in the future are suggested.

INTRODUCTION

The review is limited to models concerned with the delivery of water, sediment, plant nutrients (native or applied as fertilizer) and other agricultural chemicals to streams. The review does not cover models dealing with water quality change in streams due to in-stream processes, nor are models considered which are based solely on in-stream measurement. Models concerned with pollutant delivery to streams make use of component models often developed for and tested at a plot or field scale. Hence a section is devoted to component models.

The available models have an overtly deterministic bias, which therefore dominates this review, probably to a degree which leads to some lack of balance. The dominant concern with transport processes on the land surface is determined by the terms of reference of this review.

Despite offering considerable potential in terms of determining sources, residence times, and transit times for sediments in watersheds, the use of natural and man-made radionuclides as tracers has been omitted from this review. It could be the topic for a separate review.

MODEL COMPONENTS: THE THEORETICAL/EXPERIMENTAL CONTENT DRAWN UPON IN NPSWQ MODELS

Infiltration and Overland Flow

In the pre-ponding stage of rainfall, infiltration rate is equal to rainfall rate. At steady state the water content achieved in the soil profile above the wetting front is such that the hydraulic conductivity at that water content equals the rainfall rate. For constant high-rate rainfall (P), the time to ponding, t_p is given (Perroux et al 1981) by

$$t_p = 0.5 (S/P)^2 \quad (s) \quad [1]$$

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where S is the sorptivity (a function of initial and final water contents). Clothier and White (1981) have shown that the appropriate value of S is measured at a small suction, since macropores are unfilled prior to ponding. Estimating t_p when P is time-variable is more complex, but is approximately the time at which cumulative infiltration is $\sqrt{2}$ times the cumulative rainfall. Following ponding, surface detention (which depends on surface morphology) must be satisfied prior to the commencement of overland flow.

It follows from equation 1 that the generation of overland flow due to rainfall rate exceeding infiltration rate without requiring saturation of the subsurface soil profile is common when $P \gg S$, i.e. with high rainfall rates and/or low S (taking S to be the dominant term in infiltration rate at short times). High rainfall rates are more frequent in tropical and semi-tropical environments. In such environments Hortonian assumptions of extensive overland flow are therefore more likely to be experienced. This is far less likely in temperate conditions, where infiltration rate may commonly exceed rainfall rate, except on those regions of the three-dimensional landscape where the soil profile becomes saturated. These saturated zones will occur in draining landscapes where the subsurface flux of water moves laterally through the profile from upslope regions (for example over a deeper layer of low permeability). When the soil profile's ability to conduct that flux is exceeded, then a saturated zone is formed (O'Loughlin 1981, 1986). Overland flow may then be restricted to these saturated regions, which can expand areally during a rainfall event. In such environments, even though interest may center in overland flow, the zones where this will occur are determined entirely by subsurface flow, which therefore must be understood. If the assumptions made by O'Loughlin (1986) are satisfied, then this does not imply the need for a complete solution of subsurface water movement in all the three-dimensional space in the catchment of concern. Rather the solution can be focused on where the problem is of interest (at least for prediction of waterlogging and regions of overland flow).

Within a catchment there can be spatial variation in ponding time due either to variation in infiltration rate characteristics or to differences in the capacity of the profile to store water. Van de Griend and Engman (1985) have outlined the difficulties in using this concept in practical hydrology. Boughton (1987) has described a practical method by which the proportion of a catchment that contributes overland flow can be determined by analysis of rainfall and runoff records. The method assumes spatial variability in storage capacity, but would also apply if spatial variability was in infiltration characteristics. Analysis of surface saturation zones by topographic analysis and flow routing where appropriate (Moore et al. 1986) would be expected to provide deeper physical insight into variable source areas of runoff. The analysis of Gburek (1983) should also be helpful.

In principle all real-world generation of overland flow should lie between the upper limit of Hortonian flow and the lower limit of topographically-developed zones of saturation. High rainfall rates, low infiltration rates and exposed soil are all factors which lead toward the Hortonian concept of overland flow generation. The opposite to these factors will lead toward surface saturation zones being the major source of overland flow. This conceptual frame appears more adequate than argument about whether or not to accept the Hortonian model of overland flow (Hadley et al. 1985).

Whether overland flow is extensive (or Hortonian) or restricted to time-varying source areas of saturated soil, the question remains as to the dynamic relationship between runoff and excess rainfall rate. For a plane land surface these dynamics have been solved analytically for any time-variant excess rainfall rate (Parlange et al. 1981). A simpler approximation (Rose et al. 1983) is of the form

$$R = Q + K_1 \frac{dQ}{dt}$$

[2]

where R = excess rainfall rate (assumed uniform over the plane $[L/T]$),
 Q = runoff rate per unit area of plane $[L/T]$, and
 K_1 = constant involving length, slope and roughness of the plane.

Surface roughness can be due to soil structure, microrelief, plant residue, etc. Since by definition:

$$R = P - I \quad [3]$$

where I is the infiltration rate $[L/T]$, equations 2 and 3 can be used to determine I as a function of time under rainfall falling on a plane where the slope and length of plane (or strictly the length of ponding contributing to runoff) is known, and where $Q(t)$ is measured. $R(t)$ can then be calculated from equation 2 if surface ponding can be neglected, and, with rainfall rate also measured, $I(t)$ follows from equation 3. This methodology has the advantages over other methods of providing $I(t)$ under natural rainfall and of providing an appropriately spatially averaged value for the area contributing to the measured runoff. Campbell et al. (1984) showed that equation 2 also applies for the uniformly diverging or converging surfaces of a cone or inverted cone provided the appropriate analytical expressions are used for K_1 .

The approximate analytical solution, equation 2, is sufficiently simple that it can be readily incorporated into rainfall-runoff models without requiring extensive computer time, and Moore (1985) suggests it is therefore attractive in catchment modeling studies. Moore (1985) and Moore and Kinnell (1987) have improved the accuracy of equation 2 by generalizing a water profile shape factor assumed constant in Rose et al. (1983). The analytic correction involved improves accuracy with essentially no increase in computational complexity. Shape factors for converging and diverging planar surfaces have also been derived (Moore 1985). Similar correcting shape factors for conical or inverted conical surfaces have yet to be derived.

A potential advantage of such an approach is that the complex geometries of natural catchments could be approximately decomposed into simple, converging or diverging planar surfaces, or into converging (valley head) or diverging conical elements, for which the simple analytical solution, equation 2, applies (with appropriate values of K_1). The place, advantages and disadvantages of this approach in dealing with the complexities in surface geometry of real catchments compared to the use of 3-dimensional terrain capability and numerical solutions of overland flow is a significant but little-explored area of research.

The above discussion has focused on overland sheet flow on land surfaces. Moore and Burch (1986) have shown how the modification of sheet flow by its channeling into rills of known geometry and frequency can be dealt with making the same assumptions of kinematic flow and Manning's equation as are commonly made to describe sheet flow.

In temperate climates maximum rates of runoff may occur with snowmelt, not rainfall. Processes affecting snowmelt runoff are not dealt with in this review. Typically upland runoff concentrates into flows, whether or not this is guided by man-made structures such as graded terraces. Water needs to be routed through such networks to the more permanent channel or stream systems. Again the choice is between analytical or numerical (Brakensiek et al. 1966) methods.

Transport of Solutes Through Soil to Streams

The effect of leaching on water quality is the topic of other reviewers. Whether a more deterministic convection-diffusion model framework is used, or a more statistical framework is preferable appears to depend in part on the scale of transport involved. Leached solutes of any kind can reappear at the soil surface in the zones of saturation discussed previously. These zones are formed particularly around valley bottoms, but in general occur whenever the upslope drainage across a contour element exceeds the capacity of the soil profile to conduct the flux at that

location. In this situation, especially common in temperate environments with landforms of vertical relief and limited soil depth, solutes transported in subsurface flow will both re-appear at the surface saturation zone and also be directly discharged into streams. Solutes can exfiltrate at the saturation zone and become diluted with runoff from rainfall on the zone. The relative importance of these two mechanisms affecting stream water quality has received little attention.

In some countries (e.g., Australia) natural salt is by far the most widespread pollutant, and secondary salinization is a major concern. This is chiefly due to altered subsurface hydrology and, in Australia, has followed the replacement of perennial, deeper-rooted native vegetation by annual crops and pastures following European settlement (Mulcahy 1983, Peck 1978). There has been significant research on the relationship between water and salt movement in soil profiles, and in the chloride balance in farmed and forested catchments (Peck and Hurle 1973, Peck et al. 1981). In landscapes with hillslopes, saline surface seepage can develop on the lower hillslopes and/or valley floors. Saline groundwater levels rise slowly, intercepting streams, sometimes greatly raising river salinity (Mulcahy 1983).

The Implications of Soil Erosion and Deposition for Sediment Transport

A review of recent developments in erosion and sediment yield has been provided by Hadley et al. (1985), and of developments in soil erosion and deposition models by Rose (1985). What is attempted here is to discuss work published since these reviews.

Excluded from consideration here, but reviewed in Hadley et al. (1985), are the variety of processes involved in mass movement in which sediment moves under gravity without the primary assistance of fluid transport. This includes bankfall due to undercutting in gullies, where waterfall can also cause hydraulic erosion. Also excluded is subsurface erosion though this has some mechanisms in common with erosion of the surface soil.

With such restrictions, sediment flux per unit width of slope is the product of the volumetric flux of water per unit width and sediment concentration in the runoff water. Water flux depends on the hydrology of the situation, and concentration c on the net balance between the rate at which sediment is added to overland flow by erosion processes and its rate of return to the soil surface by deposition, which is a continuous process for all sediment with immersed weight.

Deposition

The rate of deposition of soil particles or aggregates with any particular settling velocity is given by the product of that settling velocity and the concentration of sediment adjacent to the soil surface. Typically soil possesses components with a very wide range of sizes and settling velocities. The depositability of sediment is described by its "settling velocity characteristic", the relationship between settling velocity and the fractional mass of sediment which settles with a velocity less than any particular value.

The settling velocity distribution can be determined using a bottom withdrawal tube (Lovell and Rose 1986, 1988a, 1988b), in combination with pipette analysis of sediment as sampled.

Rainfall Detachment and Re-Detachment

While deposition is the only process reducing sediment concentration, in general there are at least two different types of process which add to the concentration. The first process in time to occur is detachment of the soil by raindrop impact, which can persist even following the development of overland flow wherever flow depth does not exceed about four drop diameters. The sediment concentration resulting from rainfall detachment depends also on the rate of deposition. The rate of loss of sediment measured either from a splash cup or a small flume is typically used to determine the "detachability" of soil to rainfall. However, since the "depositability" of soil also affects these measurements, the result of these standard methods, uncorrected for deposition, is

not "detachability" as intended; rather it is something different, which might be called "erodibility", since the result obtained is an indicator of the net erosion rate to be expected under the action of the two opposing mechanisms of rainfall detachment and deposition.

Even with constant rainfall rate and surface water depth the sediment concentration (c) resulting from these two mechanisms is not constant, but typically declines with time until a dynamic equilibrium is achieved (e.g. Rose et al. 1989). This is associated with the build-up through time of a deposited layer which is coarser than the parent soil, and which is re-detached by rainfall impact. The change through time in c reflects the adjustment occurring between detachment of the original soil surface and re-detachment of the accumulating deposited layer of soil (Rose et al. 1989).

Entrainment and Re-entrainment

The term entrainment describes the initial removal of soil from its surrounding soil environment due to the mutual shear stresses which exist between overland flow and the surface across which it is flowing. Provided a threshold stream-power (the rate of working of the shear stress) is exceeded, entrainment leads to a sediment concentration and to deposition, and thus to the development of a deposited layer on the soil surface. Excess streampower is partitioned between entrainment of the original soil and re-entrainment of soil from the deposited layer. A dynamic equilibrium is reached when the deposition rate is balanced by the rate of re-entrainment of the deposited layer. At this equilibrium Rose and Hairsine (1988) show that the sediment concentration $c(x,t)$ at distance x down a plane at time t when overland flow rate is Q per unit area is

$$c(x,t) = \phi \left[x^{1/2} - \frac{3\psi}{2} \left(1 - \frac{\psi}{x^{1/2}} + \frac{\psi^2}{2x} \right) \right] \quad [4]$$

$$\text{where } \phi = \frac{F\rho S(KQ)^{1/2} \sigma/(\sigma-\rho)}{\sum v_i/I}, \text{ and } \psi = \frac{J\phi}{F\rho gS}, \quad [5]$$

F = the fraction of streampower used in entrainment/re-entrainment,
 ϕ and σ = water and aggregate densities,
 S = slope,
 v_i = settling velocity of particles in I size ranges,
 K = $s^{1/2}n$ with n the Manning's roughness coefficient,
 g = acceleration due to gravity, and
 J = the mechanical work per unit mass of soil required to remove soil in entrainment (related to soil strength).

An upper (transport) limit to c in equation 4 is given when $J = \psi = 0$, when from equation 4 $c \propto x^{1/2}$ and it may be shown that $c \propto SV$, where V is the velocity of flow (Rose and Hairsine 1988). More generally, when J (and so ψ) is > 0 , c is reduced, as is the strength of the dependence of c on slope (S) and slope-length (x). Thus the much-debated question of the dependence of c on S and x has no unique answer, it depends considerably on soil strength term J . The same concepts which lead to equation 4 also hold when rilling develops, the increased complexity being largely geometrical. A physical basis is thus provided to understand the well-known fact that rilling increases the efficiency of sediment transport when it occurs. However the prevalence of rilling is not universal, depending among other things on soil type and condition. Rill frequency appears commonly high in relatively high-silt soils common in some major agricultural regions of the USA. In such a situation it is useful and reasonably correct to identify the erosion mechanism in the limited inter-rill regions as rainfall detachment, with entrainment (or "runoff detachment") dominating in rills. This identity between surface morphology and erosion process is very widely used (Foster 1982). However this identity is not universal. Rilling is much less common or

virtually absent in some soil types and conditions, especially in tropical soils. Such a lack of rills does not imply absence of entrainment processes which dominate in rills. Also erosion between (or without) rills can be due to a variety of processes, so that the term "interrill erosion" should not be used as if it is a unique process.

Thus, to avoid confusion and allow generality it is recommended that the names of the erosion mechanisms be used in describing erosion processes, rather than use of the terms rill erosion and interrill erosion as implied process descriptors. Clearly this is not to deny the utility of the terms rill and interrill regions in describing a common erosion surface morphology.

The above discussion has been limited to bare soil. The great reductions in sediment concentration provided by plant-residue or other mulch in effective contact with the soil surface is well known if not completely understood (Foster 1982, Rose 1985, Brenneman and Laflen 1982).

Sediment Delivery to Streams

It follows from equation 4, developed for entrainment/re-entrainment in equilibrium with deposition, that a reduction in slope will lead to a reduction in sediment concentration. The additional contribution to sediment concentration from rainfall detachment is insensitive to slope. Fuller analysis shows that both the concentration and the settling velocity characteristics of sediment in overland flow are altered following a change in slope. Analysis of these changes is given for the case of graded terraces used as soil conservation structures by Foster et al. (1980) and by Rose (1985). The importance of settling velocity is now recognized and incorporated in some agricultural pollution models (e.g. Young et al. 1987). Further testing of the theory describing such changes is underway.

In broader-scale modeling of sediment transport to streams a simpler approach has commonly been adopted, either by neglecting changes in settling velocity characteristics (Burch et al. 1986), by use of a sediment delivery ratio which is inversely proportional to the path length of flow from the erosion site to the stream, or some more developed concept based on this slope and path length (Dickinson et al. 1986). For screening nonpoint-source pollution in large watersheds use is made of an increase power dependence on watershed area (e.g. Haith and Tubbs 1981). Other methods have been reviewed by Hadley et al. (1985).

Work on this problem is aided by working from both ends - the source of sediment and the receiving end. Analyzing suspended sediment concentration/discharge relationships in U.K. rivers, Walling and Webb (1982) illustrated the typical hysteretic behavior indicating apparent exhaustion effects in sediment availability operating both within multiple events or during a sequence of events. Similar behavior is exhibited at smaller scale and it would be worth exploring whether similar explanations might hold at the different scales.

Transport of Nitrogen

Losses of nitrogen (N) from agricultural land occur by several modes of transport and for several N species. Loss by leaching can be substantial (Winteringham 1977), especially for inorganic forms of N, losses being chiefly as nitrate (White 1988). Leaching losses can be modeled (Frere 1975, Rose et al. 1982a, b, White 1988), but this is the topic of another review in this Symposium. Losses of N can also be in gaseous form following volatilization or denitrification. Since the recent development of simplified micrometeorological methods of measuring gaseous losses of N their significance has been considerably clarified (Freney and Black 1988).

Losses in runoff of surface-applied nitrogen fertilizer can be significant (Haith and Dougherty 1976, Rose and Dalal 1988), but models of such runoff losses are empirically plausible (Young et

al. 1987) without being well-based, and the effect of management factors is not well understood (Dean 1983).

With the exception of nitrogen in nitrate form, or converted to gaseous forms, the loss of nitrogen is chiefly associated with the loss of sediment (Frere et al. 1975, White 1986), and this loss will be considered below. Thus the rate and mechanism of loss of nitrogen is strongly affected by the transformations between the various organic and inorganic forms of N which are continuously taking place. Thus the vast literature on nitrogen transformations and nitrogen cycling (recently reviewed in Wilson 1988) is a necessary background to modeling losses of nitrogen in the various processes briefly referred to above.

Transport of Sorbed Nutrients

If there are no enrichment effects associated with water erosion then the loss of any stable chemical sorbed to soil is given by the product of the sediment loss and chemical concentration in the soil. However enrichment effects are common. Dean (1983) identified the lack of a systematic approach to such enrichment effects. Foster et al. (1985) and Rose and Dalal (1988) illustrate how the enrichment ratio (E_R) depends upon soil types, tillage practice, the mix of erosion mechanisms, and time. Observations show that E_R declines as sediment yield increases, and increases as the clay content of soil decreases (e.g. Sharpley 1985). The decline with sediment yield is represented for example in the model CREAMS (Knisel 1980).

A theoretical framework on which to interpret the many and varied relationships affecting E_R has been provided by Rose and Dalal (1988) and illustrated by Rose et al. (1988). On this framework E_R is seen to depend on the product of two distributions. The first distribution is the settling velocity distribution of sediment, which is strongly modified by the mix of erosion mechanisms and by time or mass eroded. For example, rainfall detachment leads to higher enrichment ratios than entrainment. Selective deposition following transport to lower slopes, where finer sediment results, also affects the settling velocity distribution and thus E_R .

The second distribution involved is the relative distribution of the sorbed chemical with respect to settling velocity, a more stable distribution than the first for any given soil and (stable) sorbed chemical. The utility of this theoretical framework has been illustrated for organic-N (Rose et al 1988), but should be of general application.

Pollution prediction uses loading functions dependent on a potency factor which includes E_R and a ratio R (Dean 1983), which is the ratio of particle densities in surface soil to that in eroded sediment. This ratio R may well be involved in sediment delivery but conceptually should not be associated with a "potency factor" as is commonly the case (Dean 1983).

Transport of Pesticides (including Herbicides) With Sediment

The solubility and sorption characteristics of pesticides vary widely, and these characteristics have a substantial effect on the partitioning of pesticide loss between the sediment and water phases. Pesticides with higher solubilities in water are lost mainly in the water phase (Wauchope 1978), and those strongly sorbed to soil mainly with sediment. For strongly-sorbed, less water-soluble pesticides, the theoretical framework referred to previously should assist the interpretation of enrichment effects (Dean 1983). However for all pesticides, especially the less persistent types, chemical or biological degradation is generally the major pathway of pesticide loss. Half-lives of 10-80 days are commonly reported for less-persistent pesticides (e.g. Wauchope 1978). Though no single equation can describe the breakdown of all chemicals in any environment, a first-order rate equation often provides a useful approximation (Frere 1975, 1982). In this type of description it is recognized that the degradation coefficient depends on the pesticide and its changing environment.

Seasonal and long-term losses of pesticides from fields tend to be greatest when formulated as wettable powders for surface application; next in amount of loss are water-insoluble insecticides usually applied as emulsions; losses in runoff are usually least for water-soluble pesticides (Wauchope 1978). Water-soluble pesticides may move through sub-surface flow to groundwater and hence to streams. This slower transport route provides more time for breakdown compared to overland flow, but lack of carbon sources for bacteria could severely limit degradation, and breakdown is pesticide-dependent.

As would be expected, losses of sorbed herbicides (e.g. paraquat) are related to sediment loss, and of water-soluble herbicides to runoff volume (Leonard et al. 1979). These authors found a reasonably direct relationship between concentrations of water-transported soluble herbicides in runoff and their concentration in the soil surface.

The volatility, placement, and soil and vegetation conditions on application all affect pesticide loss. Sorption effects, while sometimes well-represented by Freundlich-type isotherms (Rao and Davidson 1980), can also be irreversible. Pesticide losses can be substantial in a single storm soon after application, and pesticide concentration in runoff can vary by an order of magnitude during a single runoff event (Wauchope 1978), indicating that within-storm time scales would be needed to interpret the processes involved in pesticide loss. It is therefore not surprising that there can be great variability in pesticide mass loads and concentrations despite strong associations between seasonal pesticide loss and runoff volume (Haith 1986).

THE INTEGRATION OF COMPONENT MODELS INTO NPSWQ MODELS

Model Types and Purposes

A partial list of agricultural nonpoint-source pollution models is given in table 1, and some of their characteristics given in table 2. Table 1 indicates that basic hydrologic models such as the Stanford Watershed Model can be used in a number of models developed to describe sediment or chemical loss. Most models have been constructed in this piggyback fashion on models of overland flow, recognizing it to be the common dominant agent of transport of sediment and chemicals to streams. This is not to deny the possible substantial importance of delivery of dissolved or colloiddally-bound forms of pollutants to streams through the groundwater system, nitrate and chloride providing examples of this.

Nonpoint-source pollution models have been divided according to purpose (Barnwell and Krenkel 1982, Novotny and Chesters 1981). Screening models which relate expected pollution loading to land use, while not intended to be precise, are useful in identifying potential problem areas in large catchments (Dickinson et al. 1984, Haith and Tubbs 1981). Screening models permit evaluation of a broad policy nature such as the identification of potential environmental problem areas; planning models focus on the development of the major features of control strategies; design models translate major features of control plans into site-specific management practices; and comprehensive models focus in great detail spatially and temporally on single pollutant impact problems for control or regulatory purposes. The models presented in tables 1 and 2 have not been specifically classified on this basis, the categories not having been distinctively defined and the models not having been thoroughly evaluated in this regard. Mathematical hydrologically-based models attempt to describe the outcome of processes, if not the processes themselves (Novotny 1986); an objective of such models is to relate catchment and environmental characteristics to system behavior.

Mathematical models can be conceptual or empirical, and deterministic or stochastic in character, though such distinctions are not precise and unambiguous (Clark 1973, Freeze 1975, and Frere

Table 1.
Partial list of agricultural nonpoint source pollution models.

Model Acronym and Name	Source/Basics	Reference
PTR-Pesticide, Transport, & Runoff	Stanford/Hydrocomp	Crawford and Donigian 1973
ARM-Agricultural Runoff Model	"	Donigian et al. 1977
NPS-Nonpoint Simulation Model	"	Donigian and Crawford 1977
HSPF-Hydrologic Simulation Program - FORTRAN	"	Johanson et al. 1984
ACTMO-Agricultural Chemical Transport Model	USDA/ARS	Frere et al. 1975
CREAMS- Chemicals, Runoff, and Erosion from Agricultural Management Systems	"	Knisel (ed) (1980)
AGNPS-Agricultural Nonpoint Pollution Model	"	Young et al. 1987
ANSWERS-Areal Nonpoint Source Watershed Environment Response Simulation	Purdue	Beasley et al. 1980
UTM-TOX-Unified Transport Model for Toxics	Oak Ridge	Patterson et al. 1983
LANDRUN-Overland Flow and Pollution Generation Model	Wisconsin	Novotny et al. 1979
GAMES/GAMESP-Guilph Model for Evaluating the Effects of Agricultural Management Systems on Erosion and Sedimentation/Phosphorus	Guelph	Cook et al. 1985
Land Directorate-Method for Targeting of Agricultural Soil Erosion and Sediment Loading to Streams	Environment Canada/GAMES	Snell, 1984
EPA Screening Procedure -	EPA	McElroy et al. 1976

Table 2.
Characteristics of selected agricultural nonpoint source pollution models.

Model	Hydrology			Erosion and Sedimentation		Chemicals			Time Scale			Space Scale			
	Surface Water	Subsurface Flow	Snow	Soil Loss	Sediment Yields/Loads	Nutrients	Pesticides	Other	Event	Continuous	Seasonal/Annual	Field	Farm	Small Watershed	Region
PTR	x	x	x	-	x	x	x	-	-	x	-	-	-	x	-
ARM	x	x	x	-	x	x	x	x	-	x	-	-	-	x	-
NPS	x	x	x	-	x	x	-	x	-	x	-	-	-	x	-
HSPF	x	x	x	-	x	x	x	x	-	x	-	-	-	x	-
ACTMO	x	-	x	x	x	x	x	-	x	-	-	-	x	-	-
CREAMS	x	x	x	x	x	x	x	-	-	x	-	x	-	-	-
GLEAMS	x	x	x	x	x	x	x	-	-	x	-	x	-	-	-
SWAM	x	x	-	x	x	x	x	-	-	x	-	-	-	x	-
AGNPS	x	-	-	x	x	x	-	x	x	-	-	x	x	x	-
ANSWERS	x	x	-	x	x	x	-	-	x	-	-	-	-	x	-
UTM-TOX	x	x	x	-	-	-	x	x	-	x	-	-	-	x	-
LANDRUN	x	x	x	-	x	x	-	-	-	x	-	-	-	x	-
GAMES/P	-	-	-	x	x	x	-	-	-	-	x	-	-	x	-
UNITED AREA	-	-	-	-	x	x	x	x	-	-	x	-	-	-	x
LANDS	-	-	-	x	x	-	-	-	-	-	x	-	-	-	x
EPA Screening	-	-	-	x	x	x	x	-	x	-	x	-	-	x	-

1982). As the spatial and time scales of interest increase, models with a stochastic rather than deterministic basis are more likely to be used.

Models can be distinguished with regard to the temporal nature of their focus, be it single storm event simulation, continuous simulation for many years, or average long-term estimation (e.g. seasonal, annual). Obviously, continuous models can also be used for single events, and if run for many months and years, for generating seasonal loads, annual loads, and average seasonal and annual loads. Also event models can be used to simulate a seasonal or annual sequence of events, but with greater difficulty and cost if the event model is complex.

The purpose of each model, the form of constraints on its structure, and its input requirements suit it for a particular spatial scale of application i.e. field, farm, small watershed, or region. As the extrapolation of information and process descriptions from a field to a watershed simulation is still fraught with many difficulties, the algorithms selected for the model and the model selected

for the problem being addressed, must be appropriate to the spatial scale of the processes of interest.

Related to the scale of application, models can be of lumped- or distributed-parameter type. In distributed-parameter models, watersheds are commonly subdivided into elements or cells assumed uniform in characteristics such as soil type, slope, and management (e.g. Beasley et al. 1980). The greater data requirements and computing time of distributed models tends to restrict their application to modeling single or few runoff events (Beasley et al. 1980, Young et al. 1987) rather than for investigating long-term behavior. Such models tend to be used for purposes such as land-use planning and management in watersheds.

Methods of Dealing with Hydrology

The commonly used methods of modeling the relationship between runoff and rainfall in catchments (whether in a rural or urbanized condition) is illustrated by the program RORB (Laurenson and Mein 1985). In this program hydrographs are computed by deducting infiltration and storage "losses" from rainfall, and routing the rainfall-excess through a model of the various catchment storages. Catchment storages include both overland flow and channel storage. Storage (S_t) is modeled nonlinearly as being proportional to the discharge (q) from a plane or channel reach raised to a power (p) so that:

$$S_t = b q^p \quad [6]$$

Both b and p have to be determined by fitting experimental data, usually on the complete catchment (Laurenson et al. 1985).

The assumption of kinematic flow (i.e. of a unique relationship between flow rate and flow depth) has been widely explored (Lighthill and Whitham 1955, Woolhiser and Liggett 1967). Such analysis has usually involved numerical solution of the characteristic equations obtained, although an exact analytic solution is available for a plane land surface or channel (Parlange et al. 1981), and simple approximate analytical solutions for a variety of surface forms (Rose et al. 1983, Moore 1985, Moore and Kinnell 1987).

What has not been as widely achieved is the potentially fruitful outcomes of connecting theoretically-rich approaches of the types outlined in the above paragraph with the experimentally-rich applications of practical rainfall-runoff models such as RORB. Such connection illustrates, for example, that the empirical relationships between water storage (on watershed elements) and discharge can be expressed theoretically. For example S_t , the storage per unit area of plane, is given by

$$S_t = C (a/K)^{1/m} \quad [7]$$

where C = a water surface profile shape factor (Moore 1985),
 a = the water flux per unit width at exit from the plane, and
 K and m are defined by the kinematic rating equation

$$q = KD^m \quad [8]$$

where D = depth of flow, and
 $K = S^{1/2}/n$ where S is plane slope and n Manning's roughness coefficient.

Thus, in this simple situation of a plane, the empirical coefficients b and p in equation 6 can be predicted from equations 7 and 8.

As an illustration of the utility of making the connection between theory and practice, in fitting hydrograph data for two catchments in Australia, Laurensen et al. (1985) drew attention to the common problem of interaction between the two coefficients b and p in equation 6, and the consequent difficulty in choosing unique values for either. Comparing equations 6 and 7 it follows that $p = 1/m$, with $m \approx 5/3$ for turbulent flow and 3 for laminar flow. Laurensen et al. (1985) explored the range 1.0 to 0.5 for p , corresponding to the range in m from 1.0 to 2.0. If flow was fully turbulent then $m = 1.7$ could be assumed. Similar comparisons could be made between the empirical factor b and its equivalent from equation 7 (for a single plane) of $C/K^{1/m}$. The slope and roughness dependence of K would clearly be a cause for variation in the parameter b . Thus the value of b obtained by fitting the watershed hydrograph would depend in part on an integration of the effect of the variety of slopes and roughnesses in that fraction of the catchment yielding overland flow.

Generalizing these specific comments it is recommended that in future hydrologic modeling cognizance is taken of the existence of simple approximate kinematic flow theory. The utility of this theory in determining infiltration characteristics was noted previously. This is important since ignorance of field infiltration characteristics is often a major limitation in the accuracy of hydrologic prediction, and thus of sediment and other pollutants.

Methods of Dealing With Sediment and Chemicals

The transport of eroded sediment to streams is clearly linked to overland flow, the magnitude of which also affects the rates of entrainment and re-entrainment as discussed in an earlier section. Thus the erosion and transport of sediment is effected by linkage with the component model dealing with overland flow, except where soil loss is estimated via the Universal Soil Loss Equation, where soil loss is related, among other factors, to rainfall rather than runoff characteristics.

The loss of chemicals sorbed to clay or organic matter is related to soil lost from the catchment, estimated with either of the two methodologies referred to in the paragraph above.

CASE STUDIES ALLOWING QUANTITATIVE COMPARISON BETWEEN NPSWQ MODELS

Case studies discussed here are restricted to those in which quantitative comparisons have been made between models using the same data set.

Hydrology

Pathak et al. (1984) compared to the performance of the USDAHL-74 (Holtan et al. 1975) and CREAMS (Knisel 1980) models in simulating monthly and annual runoff from four grassland watersheds ranging in area from 6 to 80 ha. In the USDAHL model the watershed is divided into three hydrologic response zones, whereas CREAMS is a lumped model. Thus it is understandable that USDAHL simulated monthly runoff more accurately than CREAMS on all watersheds. The models differed substantially in estimated evaporation and both were most accurate in predictions for small watersheds with relatively homogeneous soils (conditions specified as CREAMS assumptions).

Laurensen et al. (1985) compared the capabilities of three models to describe rainfall-runoff events in paired catchments of approximately 1 km^2 , a purpose being to investigate the effects of urbanization on catchment hydrology. The three models compared were RORB (Laurensen and Mein 1985), STORM (Hydrologic Research Center 1976) and SWMM (Huber et al. 1981). The hourly time increment of STORM made it unsuitable for use in these small catchments despite giving reasonable total runoff estimates. RORB fitted several hydrographs with reasonably

consistent parameter values, allowing quantification of urbanization effects which increased watershed runoff some six times. The capability of SWMM was reasonable in most but not all cases.

The characterization of the hydrologic characteristics of a small, temperate forested watershed by Moore et al. (1986) is not so much a comparison of different models as an illustration of how different models need to be combined to achieve such characterization. In this watershed the location and size of saturated, runoff-producing zones controlled the response of runoff to rainfall. The location and extent of local saturation was predicted by O'Loughlin's (1986) saturation zone model. Overland flow routing across this saturated zone was modeled using the approximate kinematic overland flow equation (Rose et al. 1983, Moore 1985). Following calibration of three physically-defined parameters, hydrographs for other events were well simulated. This combination of variable source-area identification with an analytic kinematic flow equation allows realistic and simple calculation of the quickflow contributions from saturated source areas.

Sediment Erosion and Delivery

Foster (1982) reviewed the thirteen erosion and sediment yield models available at that time. For the USLE erosion predictor commonly used in the USA, a data base on soil erodibility has been built up by calibration with a large number of experiments. The summary of this data base in a convenient form for users has been a great strength of the USLE (Wischmeier and Smith 1978). While the limitations of the USLE approach are now widely understood, it has not yet been effectively replaced for general use for two reasons. Firstly, of the alternative, more process-based erosion and sediment delivery models currently being developed and tested it is premature to make any firm recommendations concerning which is most suitable for what purposes. Secondly there is not yet established a sufficiently wide data-base so that such models can be generally used in a predictive mode.

Several models show useful abilities to fit certain sets of data. For example Yang (1972, 1976) has developed an equation making use of the concept of unit stream power which very well fits data on the transport of noncohesive sediment of any particular size, and this equation should apply well to reaches with well-sorted sand in stream beds. However it is clear that agricultural sediments are cohesive and possess a wide distribution of sizes. The work of Rose and Hairsine (1988) indicates that the behavior of such noncohesive, single-sized sediment is one extreme in sediment behavior, its rate corresponding approximately to the "transport limiting" concept of Foster (1982).

Lorber and Mulkey (1982) compared predictions of sediment loss by three erosivity models. In this comparison the model of Onstad and Foster (1975) gave better prediction of total soil loss than that of Wischmeier and Smith (1978) (which under-predicted) and Williams (1975) (which over-predicted by a factor of 2). All models over-predicted sediment loss for very large-peak events, so some degree of self-compensation must be present.

Delivery of Chemicals

A summary of the process representation in current pesticide runoff models is represented in table 3 (Mulkey et al. 1986). A complication in assessing and comparing chemical runoff models is that the properties, application procedures and formulation of the applied chemical all affect the relative importance of the various processes.

Lorber and Mulkey (1982) evaluated and compared the utility of three pesticide runoff loading models. These models were the Agricultural Runoff Management (ARM) version II, the Continuous Pesticide Simulation (CPS), and the Chemical, Runoff, and Erosion from Agricultural Management Systems (CREAMS). Comparison was made between measurement and model

Table 3.
Pesticide Process Representation in Current Pesticide Runoff Models
(From Mulkey et al. 1986).

<u>Model</u>	<u>Transport Mechanisms</u>	<u>Degradation</u>	<u>Soil-Water Partitioning</u>	<u>Plant Processes</u>	<u>Other Options</u>
PRS	Dissolved in surface runoff, sorbed to eroded soil	First order, lumped decay rate	Reversible, instantaneous, equilibrium, single-value linear isotherm	Foliar washoff and decay	Enrichment ratios
CREAMS	Dissolved in surface runoff, sorbed to eroded soil	First order, lumped decay rate	Reversible, instantaneous, equilibrium, single-value linear isotherm	Foliar washoff and decay	Enrichment ratios
CPS	Dissolved in surface runoff, sorbed to eroded soil	First order, lumped decay rate	Reversible, instantaneous, equilibrium single-value linear isotherms	None	None
ARM II	Dissolved in surface runoff Dissolved in inter-flow Sorbed to eroded soil	Time-phased series of first order, lumped decay rates	Reversible and irreversible, single and non-single valued, Freundlich isotherm	None	None
HSPF	Dissolved in surface runoff Dissolved in inter-flow Sorbed to eroded soil	Time-phased series of first order, lumped decay rates	Same as ARM II with added option for sorption/desorption kinetics	None	None

estimates of field-scale runoff of two pesticides on a monthly and annual basis. A long-term (5 year) comparison was made for toxaphene.

There are differences in these models with respect to their representation of hydrology and sediment transport. In all models pesticide degradation is represented by first-order kinetic equations. Time and space variability in such degradation is possible only in the ARM model. ARM alone had the capacity to simulate changes within a storm rather than on a storm-averaged basis.

All these models simulated monthly total runoff quite well following prior calibration or parameter adjustment. CREAMS underpredicted sediment loss. Correlation coefficients when measured monthly data were regressed against predictions in all three models were higher for runoff and sediment loss predictions than for predicted pesticide loss.

Lorber and Mulkey conclude that all three models required calibration in order to closely reproduce observed data, and that the calibration procedures required for each model were quite different, as was the degree of calibration. Uncertainties remained due to the effects of enrichment and interflow on the predictions. Long-term simulated toxaphene losses followed the same general frequency trends for each model. Insufficient data prevented the authors from evaluating the ability of any of these models to represent extreme events.

CONCLUSIONS, DILEMMAS, AND THE FUTURE

What Has Been Achieved?

With the development, testing, and preliminary application of the numerous agricultural nonpoint-source pollution models has come considerable learning about the processes involved, our ability to affect them, and our ability to model them. A few of the more significant steps in learning are discussed briefly below.

- (1) **Improved Data Bases**--The implementation of a nonpoint-source model in a selected area - be it field, farm, watershed, or regional scale - requires the collection, assembly, and manipulation of substantial amounts of data regarding a number of watershed and climatic variables. This exercise alone has facilitated the compilation and evaluation of existing data bases, helping to clarify gaps, errors, and shortcomings in the information and hence needs for improved monitoring and survey techniques.

Example: During the International Joint Commission Pollution from Land Use Activities Reference Group (i.e. I.J.C.-P.L.U.A.R.G.) modeling studies of the late 1970's, it was confirmed that there is a need for event-wise rather than just monthly sampling of variables such as suspended sediment and phosphorus in order to achieve acceptable estimates of stream loads. An initial step in this direction has been the development of the Enhanced Tributary Monitoring Program of the Ontario Ministry of the Environment.

- (2) **Identification of Critical Processes**--The calibration, testing, and fitting of nonpoint-source pollution models in a variety of situations, and the exploration of the sensitivity of model outputs to variations in input variables and parameters, have done much to clarify the most critical processes involved. It is these processes for which we have to acquire a clearer understanding or conceptual representation and/or improved input data in order to achieve improvements in our modeling capabilities.

Example: It seems very obvious, but most agricultural nonpoint-source modeling studies have confirmed the vital importance of accurately representing the infiltration of water into the soil - and our difficulty in consistently being able to simulate temporal and spatial variations in this process. Errors in estimating infiltration are carried, multiplied, and/or compounded in the subsequent determination of other model parameters and outputs.

- (3) **Confirmation of Temporal Trends**--Modeling studies have clarified and confirmed temporal patterns (sometimes initially revealed in monitored data) regarding the persistence or event-orientation of pollutant concentrations and loads. This confirmation of the expected nature of such temporal trends has provided a valuable basis for changing and improving temporal sampling strategies in data-monitoring programs, and for exploring more effective measures for reducing nonpoint-source pollution.

Example: Modeling studies in southern Ontario have confirmed that the majority of suspended sediment and phosphorus loads is transported from agricultural watersheds during a relatively short period of time involving a few runoff events in the late winter and early spring. These events are due to snowmelt runoff, a process which in this review has not received the emphasis it is due in climatic contexts where this phenomenon is important. The surface movement of pesticides occurs in an even briefer period of time in the late spring. It is now abundantly clear that accurate measurements of such loads demand sampling programs which are event-oriented and responsive; and effective pollution control measures must have major effects during these critical times.

- (4) **Insight Into Spatial Variability**--Studies involving the application of distributed watershed models have provided insights into the nature and extent of spatial variations in the processes involving agricultural pollutant generation and transport, and in the resultant pollutant yields. These results have led to fuller exploration of such topics as the characteristics of pollutant sources, the landscape and land management practices which exhibit localized and distributed sources, and the implications of spatial variability for the selection of implementation strategies for remedial measures programs.

Example: Modeling studies have revealed that in rolling upland watersheds in southern Ontario we can expect wide variations in suspended sediment and phosphorus yields from field-size areas, and that the majority of the annual loads of such variables from these watersheds emanate from a small percentage of the area. For flatter lowland watersheds, the spatial variations in sediment and phosphorus yields are much smaller. Such findings have prompted consideration of the importance of targeting remedial measures, particularly in areas exhibiting wide spatial variations in pollutant yields.

- (5) **Insight into the Possible Impact of Remedial Measures--**Nonpoint-source models have been used in a predictive mode to examine the possible impact of remedial measures on the generation and delivery of downstream pollution. Although absolute loads have usually been estimated for selected changes in soil and/or crop management practices, perhaps the most useful results to date have been provided by consideration of the possible relative effects of changing various practices. As very few of these results have been validated in the field, particularly for watershed and regional scales, even the predictions of relative effects should be viewed as preliminary estimates. Nonetheless, such model outputs have provided at least some valuable hypotheses to be explored more fully in the field.
- (6) **Insight into the Effectiveness of Alternative Implementation Strategies--**Is it more effective - technically (in terms of reducing pollutant loads) and costwise - to encourage implementation of pollution control measures by educational, financial incentive, or technical assistance programs? This is a planning level question, and it has been demonstrated that nonpoint source pollution models show promise of providing invaluable input for its resolution. As in the case of evaluating the impact of specific remedial measures, there is a need for field validation of these hypothetical results before they become generalized.

Example: In rolling upland areas of southern Ontario, where nonpoint-source pollution yields of sediment and phosphorus are spatially highly variable, it has been estimated that the targeting of significant changes in cropping practices (i.e., directed with technical assistance and/or financial incentives to such areas) to less than ten percent of the area exhibiting the largest rates of soil loss could reduce the total sediment load from the area by 25 percent. On the other hand, random implementation of moderate changes in cropping practices (i.e., encouraged with general educational and/or financial incentive programs) would be required in 85 percent of the area to achieve the same reduction in sediment load.

Some Specific Conclusions

Using the theory of O'Loughlin (1981, 1986) has significant computational advantages over numerical methods in locating the formation of saturated zones in draining landscapes. This approach efficiently defines the fraction and location of fractional areas contributing to runoff in such watersheds.

Watersheds do exist, especially in the tropics and semitropics (e.g. Bonell and Williams 1986) where Hortonian flow occurs. Thus rather than argue the adequacy of alternative views it is more productive to realize that the behavior of all real-world watersheds lies somewhere between the upper limit of the Hortonian concept of extensive overland flow without subsoil saturation and the concept of overland flow limited to saturated zones, which are often located in relation to topography or geological structures.

It is useful to recognize that the long-debated issue of the dependence of sediment loss on slope and slope-length has no universally correct answer. This dependence is strongly influenced by soil strength characteristics, even for plane slopes.

Reasons have been given why it is undesirable to use the terms rill and inter-rill as process descriptors, since the commonly assumed identity of rill and inter-rill morphology with distinct erosion processes is not universal.

Simple approximate analytic models of kinematic flow appear commonly to be adequate in describing the dynamics of overland flow on various types of catchment topography. This type of hydrologic analysis may be all that is required in problems such as evaluating the likely effectiveness of alternative soil-conserving practices. More complex numerical methods are needed to simulate expected behavior in specific complex watersheds.

What Are Our Dilemmas?

From the earlier section, What Has Been Achieved, it is evident that we have made considerable progress with agricultural nonpoint-source pollution models and their use in learning, planning, and management. However, we are faced with some substantial difficulties or dilemmas regarding their use; a few of the more pressing ones are outlined below.

- (1) **Development of Predictive Capacity**--At present, most if not all models require calibration of parameters in order to provide a good fit to behavior in any particular situation. Calibration data is not available on most problem areas, and this may always remain so. Hence the full utility of models will be achieved only when good system description results in values of parameters which can be independently measured or estimated.
- (2) **Parameter Estimation in Lumped Models**--The estimation of parameter values in the more lumped models (e.g. HSPF, GAMES) is somewhat difficult. For existing conditions (and measured data are available), the parameters can be determined by optimization or other fitting techniques. However, for prediction purposes involving changes in parameter values to represent the implementation of changes in soil and/or crop management practices, it is difficult to ascertain which parameter values to change by how much, and how changes in one parameter should be dependent on changes in another. Experience helps to resolve this dilemma; but until the parameters in parametric and semi-empirical models are more closely related to physical parameters, the dilemma remains.
- (3) **Increase in Spatial Scale**--The most effective methods of modeling nonpoint-source pollution at increasing scale, while receiving attention, is still not adequately resolved. More experience is required both at discovering the effective limitations of expanding modeling methods satisfactory at a given scale to larger scales, and the consequences of scale choice on the appropriate style of modeling.
- (4) **Parameter Estimation in Distributed Models**--There is also a problem with the estimation of parameters in distributed nonpoint-source models (e.g. ANSWERS, CREAMS), but this dilemma relates to the large number of parameters involved and the general lack of data regarding many of them. The model user is faced with the need to estimate a multitude of parameter values, and even though many are somewhat physically-based, there are insufficient data in their regard to allow ready determinations. As a result, the user resorts to employing default values, for which there is no confirmation or experience. As more data sets are assembled and tested, this dilemma will gradually be resolved.

- (5) **Input Data Requirements**--For many of the models, particularly the more detailed ones (e.g. ANSWERS, CREAMS), the input data requirements are voluminous and often unrealistic relative to data files that are readily available. This dilemma results in the estimation of input data, and the impact of errors in the input data on generated output are unknown and difficult to ascertain. Again, as more data are assembled and model-tested, the necessary precision and accuracy of input data requirements will be clarified.
- (6) **Validation of Long-term Models**--The validation of models involved with the determination of long-term average loads and patterns (e.g. GAMES, HSPF, CREAMS) is often difficult because of the long length of record required. The assemblage of long-term records and their use in model testing will gradually resolve this dilemma.
- (7) **Validation of Distributed Models**--All distributed nonpoint-source pollution models (e.g. GAMES, ANSWERS), whether parametric or physically-based, require validation of output information at a field scale. Some algorithms have been confirmed at point or plot scales, and the model outputs are often checked at the watershed outlet. However, estimated field pollutant yields or sub-watershed pollutant concentrations and loads have not been verified because of a lack of such data. This type of validation is essential if such models are to achieve and maintain credibility.
- (8) **Definition of "Design Events"**--Event models (e.g. ANSWERS) are readily validated on individual events (although they have often been found to be unpredictably inaccurate for single events), but difficult to verify on the long term, because of the horrendous requirements for data and the associated time and money involved. Because of these difficulties, there has been a desire to select a "design event" such that model studies based on this event could be considered to provide representative results for the area under consideration for the long term. Selection of such an event is indeed a dilemma! In fact, the existence of such a singular event is itself open to serious question. Yet without such a definition, the use of event models is restricted. A partial resolution of this dilemma may well be the selection of a range of events for the development of model outputs which might be considered to be representative of longer-term probabilities.
- (9) **Development of Chemical Algorithms**--Although a host of relatively new algorithms regarding the chemical pollutants, based on physical processes studied at a point in space, are becoming part and parcel of nonpoint-source pollution models, their utility at the field and watershed scales is open to question. While poor comparative results in chemical prediction is often taken to indicate that modeling the chemical component of the system is weakest, this could be mainly due to compounding errors in hydrology and sediment loss. More and better data, and a better understanding of the physical, chemical, and biological processes involved with the degradation, detachment, and transport of agricultural chemicals over and through the soil are needed.

Possible Directions and Issues for the Future

Past developments in nonpoint-source pollution models have aided the recommendation of remedial measures. In addition to seeking solutions to the current dilemmas noted in the previous section, what are other issues to be tackled in the future?

- (1) **Hydrologic Description**--Evaluation of more efficient methods of measuring infiltration characteristics should continue, and the role of surface detention in modifying runoff treated more quantitatively. The effects of change in soil type, cover and crop management on infiltration under rainfall need further investigation. The significance of

exfiltration of subsurface flow from higher land elements (as noted in saline seeps) needs better understanding, as does its quantitative comparison to interflow.

More experience with analytically-based methods of describing overland flow, and the development of topographically-related saturation zone methodology, offer promise of aiding the efficiency of describing and predicting hydrologic behavior. One example is the possibility of making use of the developments in quantitative hydrology to improve the efficiency of rainfall-runoff models. The general question of balance in the mix between analytic and numerical methods in hydrology should receive better focus in future studies, as should the mix between stochastic and deterministic modelling.

- (2) **Sediment Transport**--It could be profitable to give more attention to the various forms of mass movement of sediment, some sufficiently large-scale forms being associated with loss of life in populated areas.

A more useful database on soil erodibility under rainfall detachment could be developed if detachability and depositability were distinguished as separate characteristics. The effects of soil strength on detachability by raindrops and on entrainment by overland flow need better fundamental understanding. The possibility of usefully close relationships between the resistance offered by soil to the processes of rainfall detachment and runoff entrainment, if substantiated, could lead to more efficiency in describing soil erodibility characteristics. Likewise there may be useful relationships between the processes of re-detachment or re-entrainment of sediment deposited following the respective erosion process. Agreement on how to define and measure such soil erosion characteristics is sorely needed. When such agreement is reached then a wide data-base of such characteristics needs to be developed.

The change in both concentration and settling velocity distribution with change in land slope needs better fundamental understanding. This understanding would provide a conceptual basis for estimating sediment delivery ratios. Effects of soil management on soil erodibility, and "exhaustion" effects with repeated erosion events are aspects requiring better knowledge.

- (3) **Chemical Transport**--Improved knowledge is needed regarding the degradation of agricultural chemicals and their removal, enrichment, transport and deposition as contaminants in fields and in streams. The effect of scale and time-varying environmental factors on these processes requires better understanding. Testing concepts of the partitioning of chemicals delivered to streams between the sediment, water and biota stores is badly needed. Interactions between chemical application methods and land management have implications for chemical loss which require better understanding.

Similarities and differences in behavior with respect to loss between fertilizers and other chemicals needs further consideration so that limitations to generality of application of chemical runoff models can be better understood.

- (4) **General Issues**--Serious loss of pollutants is often associated with large events. Attention is needed on how to ensure data capture during such events and how to give proper weight to the likelihood of such events. For proper testing and validation of existing and new generations of nonpoint-source models, it is also essential that improved databases be established, including field-scale and subwatershed measurements within the context of larger watersheds. Data are needed regarding temporal variations in many of the causative/process factors, and the spatial variations in both output variables and causative factors. Some limited long-term data are needed to explore more fully the role of

extremal conditions. And to render models of more practical use, data are required regarding land management effects (on pollution), relative impacts, and costs; and information is also needed regarding the adoption of remedies in response to implementation strategies, including the relative costs associated with different strategies. The credibility of model results rests on model validation, and hence on the availability of good quality and appropriate data.

With strong, directed developments in the areas both of basic research and of data collection, application and evaluation, nonpoint-source pollution models can become more significant management and planning tools of the future.

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MODELING OF AGRICULTURAL NONPOINT-SOURCE SURFACE RUNOFF AND SEDIMENT YIELD--A REVIEW FROM THE MODELER'S PERSPECTIVE

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ABSTRACT

Modeling techniques used to simulate the hydrologic, chemical, and physical processes involved in the entrainment and transport of sediment, nutrients, and pesticides in surface runoff are reviewed. Factors affecting technique development and application, including process conceptualization and simplification, data limitations, and spatial and temporal variability are discussed. Research needs to improve simulation techniques and expand their range of applications are noted.

INTRODUCTION

The hydrologic, chemical, and physical processes involved in the entrainment and transport of sediment, nutrients, and pesticides in surface runoff are numerous and complex. Models provide a framework in which to conceptualize and investigate these processes and their interactions. Equally important, models provide a set of tools to apply the resulting knowledge for resource management purposes. Agricultural-management applications include water-resources planning, water-quality assessments, and the evaluation of best management practices.

The purpose of this report is to provide a review of state-of-the-art agricultural nonpoint-source, surface-runoff, water-quality models. Modeling approaches vary widely. They include lumped- and distributed-parameter, continuous- and event-type models for use at plot, field, and small-watershed scales. The number and diversity of models precludes an extensive comparison with respect to specific categories of models or types of applications. The common elements among these models are the system processes. Therefore, the focus of this paper will be a review of many of the approaches currently (1988) used to conceptualize and simulate the major processes affecting the entrainment and transport of sediment, nutrients, and pesticides in surface runoff. Space does not permit a detailed discussion of model-process formulations. The reader is referred to the referenced literature for specific model detail.

SURFACE-RUNOFF SYSTEM

First, the surface-runoff system and the interrelations of its water, sediment, nutrient, and pesticide related processes are briefly defined. Several processes are associated with the vegetation component of the system. Rainfall is intercepted by leaf surfaces and transferred back to the atmosphere via the process of evaporation. The leaves also transpire water from the soil profile, thus decreasing available soil moisture. Pesticide applications are intercepted by

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leaf surfaces where the chemicals reside for a period of time before being washed off to the soil surface by rainfall. During residence time on the leaves, pesticides may be lost to volatilization or to degradation by biological and chemical processes.

The soil component provides major controls on the response of the surface-water system. During interstorm periods, nutrients and pesticides may be applied and undergo a variety of transformation and degradation processes affecting the total mass of each constituent available for entrainment and transport. Land-use practices such as tillage affect the infiltration, runoff, and erosion processes.

Infiltration rates for rainfall and snowmelt are a function of soil properties, rainfall intensity, and the moisture content of the soil profile. When rainfall or snowmelt rates exceed infiltration rates, surface runoff occurs. With surface runoff comes the opportunity for the detachment and transport of sediment, nutrients, and pesticides. Nutrients and pesticides can be dissolved in surface runoff, or adsorbed or attached to sediment particles. The quantities available, the rates at which they are made available for transport, and their apportionment between the solution and sediment phases are functions of residence time, soil moisture and temperature, chemical and biological processes, and the physical characteristics of the individual nutrient and pesticide constituents.

HYDROLOGY

The entrainment, transport, and fate of sediment, nutrients, and pesticides are largely controlled by the volume and rate of water movement through and across the soil surface. Precipitation, infiltration and surface runoff are the dominant processes affecting these volumes and rates, but interception, soil-water movement, and evapotranspiration processes also are important. The complexity and accuracy of hydrology models are dependent in part on the degree to which these processes are considered.

Precipitation

Precipitation is a major driving force of the hydrologic processes, but the availability of precipitation data for many areas is limited. When data are not available or when the period of record is too short for long-term simulations, precipitation data need to be estimated. An established estimation procedure is the weather-data simulator developed by Richardson and Wright (1984) which generates daily rainfall, air-temperature, and solar-radiation data. Precipitation occurrence and amount are calculated using regionally defined parameters that can be varied by month. The Erosion-Productivity Impact Calculator (EPIC) model (Williams et al. 1984) and the Opus (not an acronym) model (Smith and Ferreira 1987) include weather-variable-generation procedures based on this simulator. Precipitation generators expand the area of application of hydrologic models but capabilities are still somewhat limited in that only daily-precipitation amounts are simulated. Disaggregation of daily rainfall into shorter-period rainfall amounts is currently being investigated (Woolhiser and Osborn 1985).

Infiltration

Infiltration controls the apportionment of precipitation between surface and subsurface-flow processes. Infiltration rate and its change with time are functions of precipitation rate, soil properties, water content of the soil profile, and surface effects, such as tillage, mulching, crusting, and freezing.

A major constraint on the detail to which the infiltration process can be simulated is the time resolution of available precipitation data. When precipitation data are limited to daily values,

more empirical modeling approaches are required. The most commonly-used approach is to estimate infiltration as the difference between daily precipitation and daily runoff, where daily runoff is estimated using the Soil Conservation Service (SCS) curve-number technique (U.S. Soil Conservation Service 1972).

The SCS procedure is used for single-event applications where antecedent soil moisture is user-defined as dry, normal, or wet. For continuous-flow simulations, the Chemicals, Runoff, and Erosion from Agricultural Management Systems (CREAMS) model (Knisel 1980) and the EPIC model use modifications to this procedure. Runoff is calculated using a curve number and a continuous functional relation based on soil-water content in the root zone. These procedures also have been incorporated in other models. The Pesticide Root Zone Model, PRZM (Carsel et al. 1985) uses the CREAMS approach, whereas the Opus model (daily hydrology option) uses the EPIC approach, which includes a stochastic runoff variation technique. Advantages of the curve-number technique include its minimal data requirements and its ease of application to a wide variety of soils, land uses, and management practices. However, its inability to account for the effects of precipitation intensity, duration, and distribution is a major source of error in runoff predictions (Smith and Williams 1980).

When hourly or shorter time interval precipitation data are available, a more detailed simulation of the infiltration process is possible. Rainfall rate, soil properties, and cumulative infiltration are the major factors that need to be considered. Some models incorporate these factors using empirical relations whose parameters are fitted using measured rainfall and runoff data or estimated using relations based on model-application experience. Other models use a physically-based approach where model parameters are estimated from measurable soil properties. The advantages of the physically-based approach lie in the hope that the parameters can be extrapolated to other locations and time periods, and that they can be applied with confidence to ungauged basins (Bevin 1985).

Models using empirical infiltration equations include the Hydrologic Simulation Program-Fortran (HSPF) model (Johanson et al. 1984) and the Areal Nonpoint Source Watershed Environment Response Simulation (ANSWERS) model (Beasley and Huggins 1982). Both models produce reasonable results, but HSPF is generally limited to applications where measured infiltration or rainfall and runoff data are available for parameter fitting. Parameter-estimation procedures and ranges are provided for the ANSWERS model, but parameters are usually fitted when measured data are available.

Many physically-based infiltration models use some form of the Green and Ampt equation (Green and Ampt 1911). Models include the Precipitation-Runoff Modeling System, PRMS (Leavesley et al. 1983), CREAMS, and the "breakpoint" option of Opus. Procedures have been developed to estimate Green and Ampt model parameters from soil properties (Brakensiek 1977, Clapp and Hornberger 1978, Rawls and Brakensiek 1983) and infiltrometer data (Brakensiek and Onstad 1977, Wu 1986). The advantages of these physically-based parameter-estimation techniques are often negated, however, by a limited ability to determine the "representative" values of selected soil properties that incorporate the spatial variability of these properties at the plot and field scale.

Accounting for the spatial variability of soil hydraulic properties is a major simulation problem. Many models use the representative-parameter approach, but it has been shown to produce substantially different simulation results than when the variability of hydraulic properties are explicitly considered (Smith and Hebbert 1979, Freeze 1980). The HSPF and PRMS models use a linear probability density function in their infiltration calculations to describe the spatial variability of soil properties. The linear assumptions are simplifications of the distribution characteristics of hydraulic variability, but have been noted as being inconsistent with the lognormal probability distribution reported for saturated hydraulic conductivity (Smith and Hebbert 1979). More

complete consideration of spatial variability will require the development of procedures that combine the probabilistic and physical descriptions of the processes.

Cultural and natural factors impacts such as tillage and surface crusting and freezing can have a substantial effect on the infiltration process. Tillage practices are incorporated in most models as discrete changes in model parameters on the dates of tillage. The U.S. Soil Conservation Service (1972) and Rawls et al. (1980) provided estimates of SCS curve numbers for selected tillage practices. Rawls and Brakensiek (1983) used soil texture and porosity change to estimate Green and Ampt model parameters associated with tillage. Evaluation of the Green and Ampt parameter-estimation procedures indicated that predicted infiltration rates and amounts had a broad scatter about their measured values (Brakensiek et al. 1983).

Surface crusting can substantially reduce infiltration rates. Most empirical models adjust for crust development by adjusting parameters. Guidance on the magnitude of these changes is very limited. The Green and Ampt equation has been reformulated by other investigators to consider surface crusting (Moore 1981, Ahuja and Ross 1983, Brakensiek and Rawls 1983), but these equations have received only limited testing and verification. The Opus model simulates the crusted profile as a dynamic two-layered system; infiltration parameters are calculated at each time step based on initial parameter estimates for each of the layers, assumed crustibility hypotheses, the moisture content of each layer, and rainfall intensity. Further testing and verification are needed to assess this approach. Limited data on crust and subcrust hydraulic properties and their spatial variability at the field scale are major constraints on these efforts.

Frozen soils may have substantially decreased infiltration rates. Two simulation problems associated with frozen soils are the determination of the presence or absence of frozen soil and the simulation of the infiltration process. Frozen soils are considered in the EPIC and HSPF models, but the equations are extreme simplifications of the processes. Additional understanding of heat and moisture movement in soils coupled with more data on soil temperature and moisture are needed to improve modeling capabilities.

Runoff

Three basic mechanisms of runoff generation have been identified from field investigations: Hortonian overland flow, saturation overland flow, and subsurface flow (Dunne 1983). Hortonian overland flow occurs when rainfall intensity exceeds infiltration capacity of the soil (Horton 1933). Saturation overland flow is generated by rainfall or snowmelt that occurs on areas saturated by the rise of the water table to the land surface. Subsurface flow is generated by the downslope movement of infiltrated water through the soil mantle.

The mix of runoff-producing mechanisms affects the quantity, quality, and timing of storm runoff. Physically-based simulations that include all these mechanisms have been limited to process investigations (e.g., Ahuja et al. 1981, Smith and Hebbert 1983). Operational applications of these runoff concepts generally use empirically-based relations. The HSPF and PRMS models simulate interflow or subsurface flow using linear and nonlinear reservoir-routing techniques. A recent modification of the ANSWERS model (Thomas and Beasley 1986) for forested applications simulates macropore and seepage flow, and variable-source-area concepts. The importance of saturation-overland and subsurface flow are recognized, but additional research is needed to improve our understanding of the processes involved. The following discussion will be limited to the Hortonian overland-flow process.

Surface runoff provides the detachment, entrainment, and transport mechanisms for the movement of dissolved and suspended materials. The temporal and spatial patterns of rainfall excess and basin characteristics (such as slope, soil type, surface roughness, and vegetation) are major factors in the determination of flow depth, velocity, and volume. Flow depth and velocity are major

determinants in the detachment and transport of sediment (Foster 1982) and in the entrainment of soluble chemicals from the soil surface (Ahuja et al. 1981, Parr et al. 1987). Entrainment and transport in surface runoff are generally assumed to occur from an effective average depth of soil and runoff-water interaction termed the EDI. In studies using tracers, the EDI has been computed to be in the range of 0.2 to 0.3 cm with the degree of interaction decreasing exponentially with depth and affected by soil aggregation, soil slope and kinetic energy of raindrops (Ahuja and Lehman 1983, Sharpley et al. 1981).

As with infiltration, the runoff-simulation approach is limited by the availability of precipitation data. When daily rainfall data are used, runoff volume is computed using the SCS curve-number technique. Advantages and errors of this procedure were previously noted in the infiltration discussion. A few models attempt to address these errors in their computational procedures. The Opus model contains the option to use a stochastic approach. This option treats the runoff estimate as an expected value rather than a prediction, and simulated storm runoff may then be distributed about this mean using a two-parameter beta distribution.

The Sedimentology by Distributed Model Treatment (SEDIMOT II) model (Wilson et al. 1981) uses the curve-number technique with precipitation type-curves that relate percentage of total rainfall to percentage of storm duration. Cumulative runoff is calculated at 3-minute time steps using cumulative precipitation calculated from the type-curves. Incremental unit hydrographs of a predefined shape are generated for each time step and the storm-runoff hydrograph is determined by convolution. Limitations of the unit-hydrograph method include the assumed space and time invariance of effective rainfall and assumed linearity in basin response (Singh 1988). However, the short time step and distributed-parameter approach of SEDIMOT II attempt to minimize these limitations.

Runoff volume provides only limited information for the estimation of dissolved and suspended storm loads. To provide an additional runoff measure, some models calculate a peak-runoff rate using the estimated flow volume and measurable basin or regional precipitation characteristics. The CREAMS model estimates peak flow as a function of drainage area, channel slope, and basin length-width ratio. The EPIC and Opus (daily option) models use time of concentration, drainage area, and a dimensionless, monthly regional-rainfall parameter to estimate peak flow. The Opus infiltration-option model calculates runoff hydrographs and thus estimates peak flow.

When short-term rainfall data are available, surface runoff can be simulated in more detail. Most storm-runoff models use the kinematic-wave approximation which simplifies the full dynamic equations for surface-water flow to a continuity-of-mass equation and a depth-discharge relation. The depth-discharge relation used in the CREAMS model is the Chezy equation, whereas the ANSWERS, HSPF, PRMS, and Opus models use the Manning equation. Surface runoff is normally assumed to occur as uniform flow over a flow-plane segment. This is a major simplification for flow planes with large surface-roughness features, such as furrows, and may be unrealistic except for extreme rainfall events.

The effects of surface-roughness features are accounted for in the roughness parameter, which is assumed to be an average value for the flow plane. Roughness-parameter values for the Chezy and Manning equations have been estimated for a variety of conditions (Woolhiser 1975). However, a considerable range of parameter values exist for each broad class of field conditions. More objective procedures are needed to characterize surface roughness and to estimate the associated roughness parameter.

The kinematic-wave assumptions are not adequate for simulating surface runoff from relatively flat slopes. For these cases, a more complete form of the surface-flow equation is needed. The Opus model uses a diffusive wave equation for simulating runoff from these flatter slopes.

Determination of where this equation is most appropriate is made using the criteria defined by Morris and Woolhiser (1980).

Water Balance

Water-balance processes are those that involve the storage and transmission of water in the soil profile. Infiltrated water moves downward through the soil profile replenishing storage and transporting nutrients and pesticides to greater depths. Water is removed from storage by evaporation from the upper regions of the soil profile and by transpiration from the root zone. Accurate accounting of soil-water storage is required because of its significant effects on infiltration rates, chemical-transformation rates for nutrients and pesticides, ground-water recharge, and plant growth.

Soil-water storage capacity is measured in terms of porosity in most models but the physical detail of water distribution within the soil profile varies. The ANSWERS model uses 1 soil zone, the PRMS and HSPF models use 2 zones, the CREAMS model uses 7 zones, the EPIC model uses 10 zones, and the Opus model allows as many as 20 zones to account for storage and water movement. Parameters used to describe the properties of these zones range from empirical coefficients in the HSPF model, to porosity measures in the ANSWERS and PRMS models, to relations between water content and matric potential in the Opus model. The more detailed models provide for greater conceptual and physical detail, but obtaining data to define the increased number of parameters and zones is a serious limit at field and larger scales.

Basin Characterization

Hydrologic response is a function of the spatial and temporal variations in basin characteristics and in meteorological inputs. Differences in modeling approaches and in model complexity and accuracy result in part from how this variability is accounted for. The spatial distribution of basin characteristics and meteorological variables is incorporated at the basin scale by segmenting a basin into subareas that are assumed homogeneous with respect to their hydrologic characteristics and response. Many models use a segmentation approach that defines free-form basin subareas using characteristics such as slope, aspect, soil properties, vegetation, and precipitation-gage location. Other uses a grid overlay to define basin subareas. The ANSWERS model uses a fixed-dimension grid of square elements, whereas the Finite Element Simulation Hydrologic Model, FESHM (Ross et al. 1978, Wolfe 1982), uses a variable-dimensioned finite-element grid.

Small grid cells may allow for a more detailed characterization, but insufficient spatial data commonly limit this advantage. Boundaries of large grid cells may not conform to topographic or land-use boundaries, thus necessitating parameter adjustments that are not well defined. Free-form segmentation procedures also result in some parameter simplification, but such procedures are more flexible and can be computationally more efficient. In all cases, the degree of geometric simplification can affect the simulated basin response (Lane et al. 1975).

Research Needs

Hydrologic models need to be applicable to a large diversity of agricultural practices at sites that generally have little or no measured hydrometeorological data. Weather-data-generation models need further development, testing, and validation to evaluate their applicability for the range of anticipated application areas, and to define and verify parameter values for these areas. Techniques to disaggregate daily rainfall into a storm hyetograph need to be developed to remove the limitations imposed on process simulations by the use of daily rainfall.

Improved techniques to estimate infiltration, runoff, and water-balance process parameters from measurable basin, soils, vegetation, and climatic characteristics are needed. The spatial and

temporal variability of these characteristics and their affect on process simulation needs to be better defined. The variability and heterogeneity of physical and hydrologic characteristics across the range of plot to basin scales also need to be defined. Investigation and resolution of these problems will require the development and application of new measurement and simulation techniques using advances in such fields as statistics and geostatistics, remote sensing, geographic information systems, and electronic instrumentation.

SEDIMENT

Water-caused erosion and sedimentation involve the processes of detachment, transportation, and deposition of soil particles by raindrop impact and runoff from the soil surface (ASCE 1975). Each of these processes is important and, under varying circumstances, any of the three may be the dominant process.

Detachment, transport, and deposition are dependent on both the meteorologic and hydrologic conditions prior to and during an event. Rainfall intensity, soil-surface characteristics, antecedent moisture, soil-tillage history, and a multitude of lesser factors all affect the movement and ultimate destination of soil particles. The physical system is quite complex and equations describing all of the possible component relations and interactions do not exist.

Modelers have used a number of approaches to simplify or rationalize the complex set of processes that describe erosion and sedimentation. Many models utilize assumed hydrologic characteristics (e.g., hydrograph shape, peak flow, and volume of runoff) as opposed to directly simulated responses. The sediment models usually are based on the assumption that detachment and deposition cannot occur in the same flow segment. In many cases, the erosion process is depicted through the use of several linearly multiplicative factors, such as in the Universal Soil Loss Equation (USLE) of Wischmeier and Smith (1978).

Many of the models presently (1988) used produce quite credible results under a variety of situations. They do what they were designed to do. Most were originally constructed to produce a reasonable result at the foot of a hillslope or at the mouth of a watershed. However, when one wishes to study the actual processes occurring in a field or at a number of places within the watershed, many of these techniques do not have the level of detail (either in structure or process relations) to meet that objective.

Thus, models of soil erosion and associated processes need to be classified as to their original purpose. There are instances of river-basin-scale models being used as small watershed planning tools. Although it may be possible to calibrate such a model for a particular situation, it is unlikely that such a model is capable of describing the processes at a scale that is orders of magnitude different than the one for which it was developed.

Detachment Processes

Soil particles can be detached by the impact of raindrops or by the shear stress resulting from overland flow. Models of the erosion process vary greatly in how they represent those processes or even if they represent them. Until about 1970, most attempts at modeling upland erosion processes involved the application of empirical representations of those processes. However, recent research has been conducted on the phenomena that collectively comprise erosion and transport. Also, the computational power available to today's researchers is orders of magnitude greater than the power available in the 1960's. Improved tools and techniques also have provided a great deal of the emphasis toward more complete process descriptions. Researchers can now use more theoretically sound and physically descriptive techniques as a result of the advances listed above.

Foster (1982) presents a lucid and complete examination of various techniques used in modeling the erosion process. He describes the two most common approaches to erosion modeling: empirically-based techniques (i.e., the USLE), and various fundamentally-based techniques that are derived from concepts and theories from erosion mechanics. The following is a condensation of the Foster analysis.

Empirical Techniques

Of the many empirical erosion equations available, the USLE of Wischmeier and Smith (1978) is by far the most commonly used. It is based on more than 11,000 plot years of data from natural and simulated runoff plots. The USLE has been applied throughout the world and is, in a true sense, the standard by which erosion estimates are judged.

The factors that comprise the USLE take into account many of the physically significant processes that occur in erosion. The R factor supplies geographic and temporal information. The L and S factors describe characteristics of the local topography. The relative erodibility of the soil is represented by K. Management (including tillage type and history, contouring, terracing, etc.) is represented by the C and P factors. All of these factors are multiplied to produce an estimate of the average soil loss over the slope length for the time period expressed in R, which is normally a year.

The USLE is a detachment-based equation (Wischmeier 1976). Deposition is not calculated, and yield from larger-scale multifield areas or changing slopes is calculated by adjusting USLE estimates using "delivery ratios" or other empirical techniques. Also, the USLE does not provide information on concentrated flow phenomena, such as channel or gully erosion.

The USLE was not designed for single-event predictions. However, Foster et al. (1977) produced a modified R factor for making more accurate, short-term estimates. A number of other modifications have been made to the USLE in an attempt to either increase the range of applicable situations or to improve prediction accuracy. Foremost among these is the Modified USLE (MUSLE) of Williams (1975). This equation utilizes runoff characteristics (volume and peak flow) of a particular watershed to produce single-storm sediment-yield estimates. The CREAMS and SEDIMOT II models contain USLE components and, as a result, generally do not require the degree of calibration of many of the other models. However, the limitations are as noted above.

Fundamentally-Based Techniques

The advantages of fundamental models compared to their empirical counterparts include the facts that they are generally more physically based and can be more accurately extrapolated, can account for spatial diversity better, can account for deposition processes directly, and can account for channel erosion and deposition (Foster 1982). Models based on fundamental principles generally require calibration because many important parameter values may not be available a priori. Several recent models attempt to use physically measurable characteristics directly in the model formulation. However, even commonplace characteristics are commonly expressed as ranges (not specific values), which leaves the modeler and model user in an awkward and generally untenable position.

Typically, fundamental models distinguish between erosion caused by raindrop impact (interrill) and by shear stress from surface flow (rill). A commonly used interrill-detachment relationship uses rainfall intensity raised to a power, a soil-erodibility factor (generally the USLE K factor), and a coefficient (Meyer and Wischmeier 1969). The rainfall power term is assumed to be 2.0 in the ANSWERS and Opus models, whereas the HSPF and PRMS models treat the term as a model parameter. The effect of rainfall intensity on interrill detachment is included in the CREAMS model using a storm-erosivity relation defined as storm energy times maximum 30-minute rainfall intensity (Foster et al. 1977).

Rill detachment is calculated directly from flow and land surface characteristics in the ANSWERS and CREAMS models, whereas other models use a transport-capacity-deficit relation. The PRMS model relates rill detachment to the difference between transport capacity and current transport rate; the Opus model uses a relation of potential rill-detachment rate to transport capacity.

Some of the more complete hydrologic models (e.g., the ANSWERS model by Beasley et al. 1980) do not have complete erosion models. The ANSWERS model, for instance, does not presently (1988) include channel erosion in its list of capabilities. Thus, potential users need to be certain of the processes they intend to simulate, and then pick a model that includes those processes.

Transport Processes

A number of simple models, like the USLE, do not directly calculate transport. Thus, sediment delivery and deposition have to be estimated by ratios that generally are inaccurate, or by other approximation techniques.

Alonso et al. (1981) presented an excellent review and comparison of eight of the most commonly utilized transport equations. Although all the equations were developed for streamflow conditions, a number are routinely used to describe sediment transport in shallow surface runoff. Obviously, flow rates, particle sizes, and even particle densities in surface runoff can be quite different from those that occur in channel flow.

Four of the equations that Alonso et al. (1981) compared were total-load equations, whereas the other four were bed-load equations. Generally, the total-load equations of Laursen (1958) and Yang (1973) and the bed-load equation of Yalin (1963) were more appropriate in a majority of circumstances. The equation of Yalin (1963) is used as the basis for calculating transport capacity in several models including the ANSWERS, CREAMS, and FESHM models. In the HSPF model the transport capacity is implicit in the interrill and rill detachment equations.

Research Needs

Although the models described above are some of most commonly used and most developed erosion/transport models in use in the United States today (1988), there are a number of processes that none of them simulate adequately. Simulations of channel erosion and ephemeral gullies are not included in most models. Simulation of interrill and rill erodibility has, until recently, always been represented as being equal.

The Watershed Erosion Prediction Project (WEPP) now being conducted by USDA-ARS is attempting to provide some of the component relations and physical descriptors that will be needed to address these and other factors. The models to be developed will address several ranges of scale and complexity. Expert-systems technology will be used to help users produce input-data files and interpret results.

Remote-sensing technology, when combined with geographic information systems, can provide much of the needed information for spatially descriptive erosion/transport models. Research needs to be increased on merging the technologies of hydrologic and erosion simulation with artificial intelligence and spatial-data acquisition and storage.

NUTRIENTS

Hydrologic and erosion processes control the extraction, entrainment, transport, and dilution of nutrients in the surface-runoff system. Chemical processes control the types, forms, and amounts of nutrients available for transport, and control their partitioning between the water- and

sediment-transport phases. Modeling the nutrient components of the surface-runoff system entails the coupling of one or more chemical-process simulations with selected hydrologic and sediment models discussed above. Chemical processes involving nitrogen (N) and phosphorus (P) are the primary nutrient processes in surface runoff and are the focus of this section. The potential for contribution of nutrients from subsurface-flow processes are recognized, but not considered in this review.

Chemical Processes and Their Interactions

Chemical processes control the proportion of the nutrient fractions in the surface-soil layer, the transformation rate between these fractions, and the transfer rate between solution and sorbed phases at interstorm and intrastorm time scales. Both N and P exist in fractions that range from soluble and reactive to insoluble and practically nonreactive. The soluble N (NO_3 and NH_4), sorbed N (NH_4), and P (PO_4 and soluble P) fractions are dissolved, diluted, and adsorbed or desorbed within the storm time scale. The organic N, organic P, and mineral P fractions move intact with the eroded materials. Total nutrient loss is controlled by the magnitude of runoff and erosion generated, the depth and efficiency of extraction from soils, the desorption rate, and the quantities of soluble and sorbed nutrients available.

The transformation rates during the interstorm periods control the nutrient quantity in each fraction and the redistribution among fractions of all nutrients from fertilizers, manure, and crop residue. Transformation rates for the organic N, organic P, and mineral P dominated fractions range from those sufficiently reactive to produce substantial NO_3 , NH_4 , PO_4 or soluble P within a relatively few days to those that occur at much slower rates. Between storms, the rapidly degradable or chemically reactive components of the organic and mineral fractions can resupply the temporarily depleted soluble and sorbed fractions. Under certain conditions, NO_3 can be lost rapidly by denitrification.

To simulate nutrient losses in surface runoff, models need to address:

- (1) the magnitude, transport, and redistributions of the water soluble, sorbed/desorbed, and sediment-attached nutrients at the storm time scale; and
- (2) the magnitude and transformation of the different nutrient fractions at the interstorm scale.

The key chemical processes that need to be considered are the ones that control solution, sorption, and transformations between fractions.

Solution and Sorption Processes

By definition, the dissolved phase includes all inorganic and organic N and P forms that pass through a 0.45-mm filter. For N, this commonly includes the NO_3 fraction, the soluble NH_4 fraction, and soluble organic N. The NO_3 losses in surface runoff are usually small and are largely controlled by hydrology rather than by chemistry because NO_3 is completely and readily soluble. Pre-runoff infiltration transports most NO_3 below the effective depth of soil and runoff water interaction (EDI). The NH_4 concentrations and losses in solution are usually small and are controlled by dilution as well as by the NH_4 sorbed to the soils by the cation-exchange capacity (CEC) of the soils. The soluble organic N fraction is usually small and is not well defined. Most of the total N lost in overland flow is not soluble, but is sediment associated, sediment intact, or particulate.

The characteristics of the dissolved P phase are similar to those of the dissolved N phase, but there are exceptions. Similar to NH_4 , the dominant PO_4 component usually is sorbed to soil, but to the uncharged mineral surface rather than by the CEC. The dissolved PO_4 concentration and

load are controlled by the sorption relation, the quantity of surface runoff, and the ratio of suspended sediment to solution in surface runoff. Exceptions that provide large dissolved- PO_4 concentrations in surface runoff include plant leaching, intense rainfall soon after surface application of fertilizers and manure, and very high P soil fertility levels.

In addition to PO_4 , the dissolved P phase contains organic and inorganic P forms that can be important, but that do not appear to be strongly sorbed. The downstream delivery of the dissolved P phase relative to all other P forms and fractions varies, depending largely on the erosion rate. Generally, where erosion rates are large, most all P transport will be sediment-associated P. Where surface-runoff volumes are large relative to erosion, the dissolved P in runoff can be dominant.

The solution process is simulated at a number of levels of detail. The ANSWERS model (Storm et al. 1988) simulates only soluble and desorbable P within the EDI. Extraction and transfer to surface runoff is based on a diffusion-controlled desorption equation. The Agricultural Runoff Management (ARM) model (Donigian and Crawford 1976a, Donigian et al. 1977, Donigian and Davis 1978) and the EPIC model simulate the solution of both N and P. The Opus model considers N and P in the EDI as well as soluble N and P washoff from the plant canopy and surface residues. In addition, the Opus model partitions soluble N and P fractions between infiltrate and surface runoff.

Sorption controls the distribution of NH_4 and PO_4 fractions between the soluble and sorbed phases. Conditions favoring formation of the sorbed phase include sorptive soil materials and large soil-to-water ratios. Under these conditions, most of the NH_4 and PO_4 will move with the suspended sediment rather than in the surface runoff. The sorption isotherm, which relates the two phases at chemical equilibrium, usually takes the form of a CEC equation for NH_4 and a linear or curvilinear (Freundlich, Langmuir) equation for PO_4 .

Under equilibrium conditions, the extent of P sorption can be computed from the sorption isotherm. For the nonequilibrium system, where the errors in assuming equilibrium are quite large, the PO_4 sorption rate is controlling and needs to be computed. These sorption rates may be quite different, depending on whether adsorption or the usually slower desorption is controlling. If the hydrologic- and erosion-process rates are rapid relative to PO_4 desorption rates, the sorption process may need to be described in terms of adsorption-desorption kinetics.

Computational methods used to simulate the solution and sorption processes vary greatly among models. The Non-Point Source (NPS) model (Donigian and Crawford 1976b) combines a "potency" factor with sediment loss to estimate total N and P losses. Loss estimates include the sorbed fractions, but do not include the soluble fractions. The CREAMS model also uses sediment loss to calculate sediment-associated nutrient loss, but has the user define the N and P content of the soil EDI, and uses an enrichment ratio to correct for particle-size selectivity in the erosion process. In addition, the CREAMS model calculates solution-phase losses as a function of user-defined soluble N and P in the soil EDI, runoff rate, and an extraction coefficient. However, the soluble and sorbed phases are not linked through kinetic or equilibrium relations. The CREAMS and NPS models are event-type models and, thus, estimates of soluble, sorbed, and other nutrient fractions in the EDI are user-defined at the start of each storm.

The HSPF and ARM models estimate the soluble NO_3 fraction, soluble and sorbed NH_4 and PO_4 fractions, and total and organic N and P fractions in overland flow. The HSPF model incorporates a slightly expanded version of the ARM model. The soluble-sorbed redistribution of NH_4 and PO_4 is described kinetically using first-order rate equations for the interstorm period only. All nutrient concentrations and distributions at the start of a storm are considered fixed for an EDI, causing the losses simulated during the storm to be physically, not chemically, controlled.

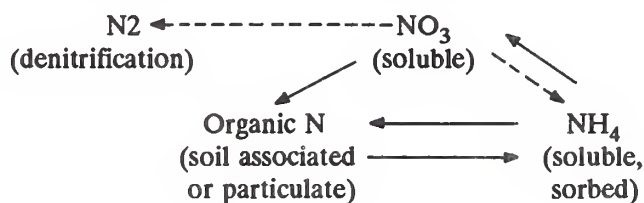
However, the HSPF model includes an option for the use of the Freundlich isotherm to calculate the sorbed- and soluble-phase concentrations.

The ANSWERS model calculates the redistribution of PO_4 between the sediment and water phases by first extracting PO_4 from the EDI using a diffusion-controlled desorption equation and then distributing this PO_4 using the Langmuir sorption isotherm. Sorption isotherms also are used in the EPIC model to distribute PO_4 , and in the Opus model to distribute NH_4 and PO_4 , between the soluble and sorbed phases. Both models include the labile-P fraction and EPIC uses this fraction in the EDI to control the soluble-P loss (Williams et al. 1984).

Transformation Processes

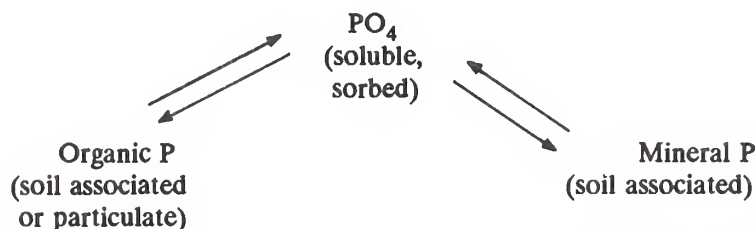
Transformation processes control the rate and amount of nutrient redistributed between fractions when one fraction is subject to a nutrient withdrawal or addition. The process type and rate depend on the nature of the fractions. Process rates are usually slow enough that the processes are much more important during interstorm periods than during intrastorm periods.

For N, the NO_3 and NH_4 fractions are considered separate fractions. The remaining organic N fraction is much larger and may be subdivided on the basis of degradability into several fractions or be treated as one. The relation for soil N is most simply constructed as:



The dominant transformations are designated by solid arrows. The organic N pool includes manure, crop residue, the microbial mass, and soil organic matter. Substantial proportions of the manure, crop residue (depending on the C:N ratio and crop), and microbial mass are more readily degradable, usually at mineralization rates ranging from days to weeks depending on climatic conditions. Fertilizer additions and crop uptake directly affect the NO_3 and NH_4 fractions. Denitrification and leaching directly affects the NO_3 fraction. These transformations and rates are microbially controlled rather than chemically controlled.

For P, there are basically three fractions: PO_4 , organic P, and mineral P, although the latter two are usually lumped together. Thus, the relation for soil P is most simply constructed as:



The PO_4 fraction includes soluble and sorbed PO_4 and could be relabeled the labile P fraction if the sorbed PO_4 is re-defined to be that desorbable during a 24-hr period. Both the organic and mineral P fractions vary considerably with respect to reactivity and degradability. Most plant or algae-available P usually is contained in these two fractions. Reactions related to the mineral P fraction are mostly inorganic and interconvert PO_4 with the strongly sorbed, amorphous, and crystalline P forms. Reactions related to the organic P fraction are microbiologically catalyzed. This fraction includes manure, crop residue, the microbial mass, and soil organic matter.

Similar to the N system, the P redistribution rate among the fractions varies, but is much slower for the more stable fractions or subfractions. P fertilizer additions and plant uptake affect the PO_4 fraction most quickly and directly. However, in soil known to be "phosphorus fixing" or "phosphorus starved", a large part of PO_4 additions can be rapidly converted to the mineral P fraction. No models currently consider the "phosphorus fixing" process.

Transformation processes affecting nutrient losses in surface runoff are incorporated in the EPIC, Opus, HSPF, and ARM models, but are not included in the CREAMS, ANSWERS, or NPS models. The HSPF and ARM models simulate the NO_3 , NH_4 , PO_4 , organic N and P, and total N and P fractions for interstorm periods.

Modeled interactions include plant uptake of N and P, denitrification of NO_3 , transfers of NH_4 and PO_4 between sorbed and soluble phases, and the N and P transformations shown above.

The EPIC model provides one of the most detailed and complete simulations of N and P fractions and their transformations. The N transformation part of the model includes N uptake separately for plants and micro-organisms, and the mineralization of organic N separately for fresh organic N, the microbial biomass, and soil organic matter. There are algorithms to compute N gains and losses by denitrification, legume fixation, plant uptake, and fertilization. However, the NH_4 fraction is not explicitly included. The P transformation part of the model includes mineralization, immobilization, and mineral P cycling components that are subdivided as well (Jones et al. 1984). Several of the P fractions are further subdivided: organic P-- fresh and stable; and inorganic P-- stable and active. Whereas the N transformation part of the model is keyed to NO_3 in the root zone, the P transformation part of the model is keyed to the labile P fraction, which lumps all soluble P with that desorbable during a 24-hr period.

In the Opus model, N and P transformation are keyed to a carbon-cycling component that defines 5 soil-carbon fractions plus crop residue in terms of turnover rates, ranging from 0.5 to 1000 years. The relations and parameters used to describe carbon decomposition are based on the assumption that microbial activity is controlling. The N-cycling part of the model is tied in by use of C:N ratios and incorporates soil and legume N fixation, denitrification, volatilization, and plant uptake. The NH_4 fraction is explicitly included. No detailed information is yet available on the P cycling component. The Opus model is a dynamic model that uses the interaction between nutrient pools and transfer/transformation processes to correct concentrations, storages, and conditions for the next time step. A major limitation of simulation at this level of detail, is that some parameters and input data for which little experience and information are available, need to be estimated.

Research Needs

The most detailed models that incorporate the latest technologies and concepts generally are technically most defensible, and, because of the detail, probably provide the most options. Practically, however, these may not be the most useful models for those needing to make farm-management or land-use decisions, given the detail and data requirements. Thus, the following research needs are targets for nutrient modeling that would provide generally useful advances.

Kinetics need to be incorporated for some nutrient fractions and relations because runoff and adsorption/desorption processes occur at similar time scales, and because desorption rate can control NH_4 or PO_4 entry to surface runoff. Transformation rates of more chemically or biologically active fractions can be fast and, thus, control the size of the nutrient pools most susceptible to loss. In addition more dynamic models need to be developed. Commonly, rapid changes imposed by a storm or a management act have important and immediate feedback effect on other nutrient pools, nutrient exposure, or conditions throughout the system.

Interstorm transformation rates for the more active N and P cycle fractions need to be included in management models. Simulating the effect of fertilizer type and timing on simulated losses in surface runoff would be most effective if management models had the capability to re-distribute the application as a function of time.

Simulation models need to be tested and validated for critical periods or conditions. Major nutrient losses in surface runoff are episodic and/or conditional. The timing, extent, and duration of exposure caused by practices, such as cultivation or surface-fertilizer application, define the most critical periods. The capability of models to simulate these changes needs to be validated. Coupled with testing, improved methods of parameter estimation need to be developed. A lack of useful and reasonable methods for estimating nutrient parameters may be the most serious limitation to nutrient simulation.

PESTICIDES

Entrainment of pesticides in surface runoff is a complex process that is extremely difficult to define in terms of rigorous mathematical descriptions of the many physicochemical processes involved. Further complicating rigorous description are the many pesticides with markedly different properties that are applied in diverse management systems. Modeling pesticide entrainment and transport would be greatly simplified if only one chemical species was involved and always applied or present uniformly in the system. Success in simulating pesticide runoff is affected by the ability to cope with the diverse chemistry of the pesticides as much as it is affected by ability to accurately simulate the hydrologic and sediment-transport systems. Simplification in the hydrology and sediment-transport submodels are sometimes made for pesticide transport in order to maintain balance in resolution among the various model components. Discussions to follow concern general models and may not include models developed for condition-specific or species-specific application.

Pesticide Dissipation at the Soil Surface

In the soil/watershed system, the primary state variable affecting pesticide entrainment is the amount of pesticide available in the effective depth of soil-and-runoff-water interaction (EDI) (Leonard et al. 1979, Mills and Leonard 1984). Models, therefore, need to adequately represent those processes that determine this pesticide mass. Application rates and methods determine the initial mass and its distribution between the crop canopy or crop residue and the soil. Pesticide residue availability during runoff is dependent on prior rates of dissipation from both the canopy and the soil surface.

Processes contributing to pesticide dissipation are volatilization, photolysis, chemical and biological degradation, plant uptake, and leaching from the soil EDI by infiltrating water. Each of these processes differ in their relative contribution depending on the particular pesticide in question. No operational pesticide-runoff model simulates all these processes independently. Most models simulate pesticide dissipation as a lumped first-order process (Donigian et al. 1977, Leonard and Wauchope 1980, Steenhuis and Walter 1980). Experience and data analysis have indicated, however, that a single first-order rate constant does not accurately represent dissipation during the entire period of persistence (Smith et al. 1978, Nash 1980, Wauchope and Leonard 1980). For most pesticides, dissipation is more rapid soon after application.

In testing and calibration of the ARM model, Donigian et al. (1977) determined that a stepwise first-order equation (different rate constant for initial and later periods) gave adequate representation of field measurements. The stepwise first-order equation also is used in the PRZM model and, perhaps, represents a reasonable compromise to maintain model balance. In the CREAMS model, only a single first-order function is used for foliar-and soil-applied pesticide.

However, foliar- and soil-pesticide pools were maintained separately so that different rate constants could be used for each. In contrast to the stepwise approach, only one rate constant was used for each pool because the critical runoff period for most pesticides is soon after application where the first substantial runoff event contributes much of the pesticide loss in runoff for the year. Also, data generally are not available for many pesticides to allow intelligent segmenting of the first-order dissipation function.

Pesticide dissipation rate also is a function of soil temperature, soil-water content, and other soil-environmental variables as outlined by Nash (1989). Where data are available, functional relations can be developed for many of those variables and incorporated into models (Hebson and DeCoursey 1989, Smith and Ferreira 1989). Work by Walker and coworkers (e.g. Walker 1978) has demonstrated the utility of soil-water content and temperature relations for a limited number of pesticides. An extensive data base, as suggested by Nash (1989), will be needed before models can make routine use of the more detailed dissipation relations. In the meantime, models will continue to use dissipation-rate constants or "environmental half-lives" derived from either field or laboratory measurements also contained in files and data bases (Nash 1989). The estimated range of error in selecting degradation-rate constants from literature sources for a given model application is within a factor of 2 (Rao and Davidson 1980), provided judgment is used in selecting those determined for similar soils under similar conditions.

Prediction of pesticide dissipation from foliage also contains considerable uncertainty (Willis and McDowell 1987). Use of simple first-order kinetics (Leonard and Wauchope 1980, Carsel et al. 1985, Leonard et al. 1987) does not allow consideration of the many variables involved. Not all pesticide-runoff models even simulate foliar sources of pesticides (e.g. Donigian et al. 1977). Volatilization and photolysis is an important pathway of foliar dissipation and models simulating the effects of weather variables would be extremely complex and require more information than is normally available.

Simulation of pesticide flux from plant foliage to the soil surface is based on empirical measurements with little consideration of type of foliage, pesticide formulation, or weather variables. The CREAMS, PRZM, and Ground-water Leaching Agricultural Management Systems, GLEAMS (Leonard et al. 1987) models use an input parameter specifying the rainfall-washable or extractable fraction of the total remaining. The CREAMS and GLEAMS models allow complete removal of the washable fraction by a step function when rainfall is in excess of canopy storage. The Opus and PRZM models use washoff functions dependent on rainfall volumes.

Process of Pesticide Entrainment/Extraction

Processes of entrainment/extraction of pesticides from the soil surface into runoff are extremely complex as conceptualized (Bailey et al. 1974; Leonard and Wauchope 1980, Leonard 1988); mathematical descriptions in terms of fundamental physicochemical processes involved would be impractical. Modelers have sought some definition of the EDI. Early models were based on the assumption that soil erosion was the dominant contributor to chemical entrainment--surface runoff equilibrating with transported sediment, or the in-situ soil solution equilibrating with surface runoff (Huff and Kruger 1967, Crawford and Donigian 1973, Bruce et al. 1975). Others have used the concept of a "mixing zone" or EDI in which concentrations in surface runoff were assumed equal to those in this mixing zone. Assumed depth of the EDI usually varies from 1 cm (Williams and Hann 1978, Steenhuis and Walter 1980, Haith and Tubbs 1981) to 0.3 cm (Crawford and Donigian 1973).

In development of the CREAMS model, a depth of 1 cm was chosen as the source zone for pesticides in surface runoff, but no depth of actual interaction was assumed. Instead, an additional parameter, an "extraction ratio", was defined as the ratio of soil mass to water mass at the soil-runoff water interface. Extraction ratios in the range of 0.05 to 0.2 were determined to

provide a reasonable fit of experimental data (Leonard and Nowlin 1980). Conceptually, this ratio was envisioned as a variable depending on soil properties, rainfall properties, and surface-runoff rate, but data have been unavailable for statistical evaluations. In the GLEAMS model, the extraction ratio has been made a function of pesticide mobility.

Pesticide Partitioning Between Soil and Water

Regardless of how the nature of the soil/surface-runoff interface is defined, some mechanism needs to be used to partition pesticides between the soil, entrained sediments, and surface runoff. The Freundlich equation, $S = K_d C^N$, or some modification of this basic equation is used almost universally in current (1988) models to partition pesticide to the adsorbed phase (S) as a function of solution-phase concentrations (C). The constants (K_d) and (N) are specific to the particular pesticide and soil (or sediment) combination. Most models also are based on the assumption of a linear Freundlich relation throughout the pesticide-concentration range normally encountered (i.e., $N=1$) such that $S = K_d C$.

Because the primary adsorber of non-polar pesticides is organic material, the equation may be rewritten as $S = K_{oc} C \cdot OC$ where $K_d = K_{oc} OC$; OC being the fraction of organic carbon in the soil or sediment. The K_{oc} is independent of soil and dependent only on the particular pesticide. These simplifications are primarily for operational expediency. Use of the linear relation also entails assumptions about reversibility and singularity and whether equilibrium is instantaneous. The CREAMS, PRZM, and GLEAMS models are based on the assumption of instantaneous reversible equilibrium. The ARM model considered a non-single valued isotherm as an option, but no marked improvement was evident compared to using the single-valued isotherm option. The Opus model provides for non-equilibrium or kinetically-retarded desorption.

Errors associated with assumptions of singularity are probably within a factor of 2 to 3 (Rao and Davidson 1980). Values tabulated for K_{oc} determined by different investigators or methods for the same pesticide commonly vary in this same range (Green and Karickhoff 1989). For a meaningful consideration of non-singularity and desorption kinetics in models, site-specific determination of necessary parameter values will be needed. Additional research is needed to provide a better understanding of the adsorption-desorption process before models can routinely simulate desorption kinetics and complex isotherms. For example, from the data of Smith et al. (1978) the apparent K_{oc} for some pesticides increased from storm to storm throughout the growing season. The same trend can be obtained from other data. As a result, models using a single value of K_{oc} to match the early storms will underestimate pesticides in sediment later in the season. However, no systematic research has been done to isolate the important variables associated with this apparent increase in adsorption (decrease in desorption) with time.

In addition to affecting the distribution of pesticides between the water and adsorbed phases, the K_{oc} affects the total amount of pesticide entrained. For relatively non-adsorbed pesticides (those with a small K_{oc} value) a substantial proportion of the pesticide is leached to greater soil depths during initial rainfall, thereby decreasing pesticide-runoff potential. This effect is magnified in soil with high infiltration rates. As K_{oc} increases, total pesticide entrained tends to increase until the amount desorbed is negligible compared to the adsorbed phase. Although these conclusions can be generally confirmed from published data (Leonard 1988), data from comparative studies in controlled experiments are lacking.

Sensitivity to K_{oc} and pesticide half-life as expressed in the CREAMS and GLEAMS models is shown in figure 1. Simulations were performed for hypothetical pesticides with combinations of K_{oc} and half-life shown using a 50-year climatic record. Surface pesticide losses reported are annual means for the 50-year period of record. Details on these simulations and simulations for a Bonify sand are presented elsewhere (Leonard and Knisel 1988). The PRZM model would be less

sensitive to K_{oc} , because the surface soil layer would probably be defined as greater than 1 cm. In the Opus model, less sensitivity to K_{oc} values could be achieved by kinetic limitations on desorption.

Stream Basin Models

The discussions above pertained mainly to development of field-scale models for application to homogeneous management units. However, these concepts also provide the basis for basin-scale models. The Pesticide Runoff Simulator (Computer Sciences Corporation 1980) was developed for application to heterogeneous basin units and is based on assumptions and concepts similar to those in the CREAMS model. The Small Watershed Agricultural Model, SWAM (DeCoursey 1982) uses the Opus model as the field unit. The HSPF model simulates in-stream processes as well as surface runoff and uses the ARM and the Pesticide Transport and Runoff (PTR) (Crawford and Donigan 1973) models to provide the pesticide functions for pesticide entrainment. The HSPF model is an excellent example of models requiring extensive data bases for calibration. Development, testing, calibration, and application of pesticide models at stream-basin scale is severely hampered by lack of data bases.

In view of the many simplifying assumptions in current pesticide models and uncertainties in values of input parameters (that is K_{oc} , degradation-rate constants, etc.) and the difficulty in validation with field data (Leonard and Knisel 1989), no model can be used to predict absolute

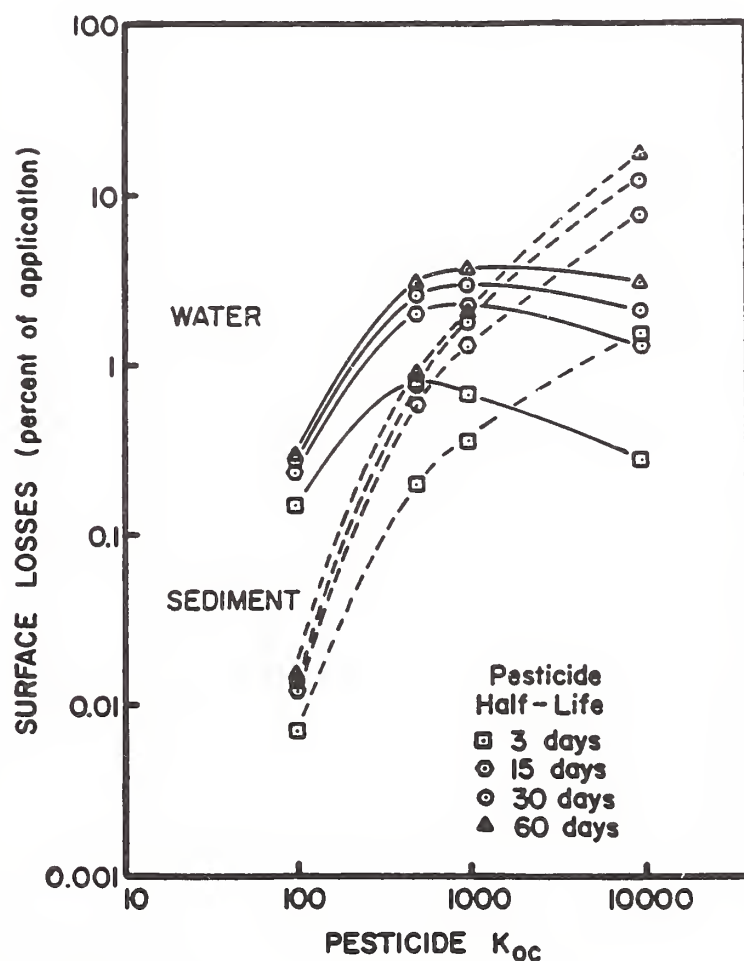


Figure 1. Pesticide runoff losses, water and sediment phases, from Greenville Sandy Clay Loam as simulated with the GLEAMS model. 50-year mean for period 1936-1985 at Tifton, Georgia.

quantities with proven accuracy. Their best use is for comparative analysis. By comparative analysis, we mean comparing different scenarios or combinations of pesticide/soil/management/climate and basing decisions on relative rankings of effects of interest.

Research Needs

For basin-wide or regional applications, simulating every field in the basin and routing field-edge outputs to some point may be impractical. Techniques to further generalize system descriptors without decreasing sensitivity to important field-scale variables, such as soil properties and management systems, are needed. In contrast, present field-scale models may not provide the resolution needed for testing system hypotheses in a research mode. For a research model, needs exist to improve our understanding and representation of: (1) pesticide persistence/dissipation as affected by edaphic and environmental variables, (2) pesticide adsorption/desorption theory, and (3) mechanisms of pesticide entrainment in runoff in relation to soil surface and foliage/crop-residue characteristics.

The dissipation process needs to be disaggregated into the individual processes of photolysis, chemical degradation, biological degradation, leaching, volatilization, and any other pathway of loss from the soil surface. Improved understanding of adsorption/desorption processes is needed to support development of non-equilibrium or kinetic representations that can be made sensitive to critical soil, pesticide, and environmental variables. For pesticide entrainment, the effects of surface roughness, particle aggregation, presence of crop canopy and crop residue, and other factors on the determination of the soil EDI need to be defined. Empirical "extraction" coefficients need to be replaced with formulations that reflect the effects of major variables such as slope, rainfall intensity, peak runoff rates, and management effects, particularly those effects of tillage and crop-residue management.

SUMMARY

Numerous models and modeling techniques have been developed to simulate the hydrologic, chemical, and physical processes involved in the entrainment and transport of sediment, nutrients, and pesticides. The number and variability of available models reflects the diversity of application objectives, differences in process conceptualization, and constraints on the types, amount, and quality of available data.

These models demonstrate the advances that have been made in the modeling of nonpoint sources in the past few decades. The advances are the result of an improved understanding of the processes involved, and the development of new technologies in the areas of data collection and computers. However, much work remains to be done to improve nonpoint-source modeling capabilities for the considerable range of problems to be addressed. Some of the improvements are very process-specific as discussed above. However, there are a number of problems that are common to all the processes; solution of these problems would help to advance the field of nonpoint-source modeling.

A more physically-based understanding of surface-runoff processes and their interactions is needed. Most proposed nonpoint-source model applications are for areas with little or no measured rainfall and runoff data, thus, parameter fitting is not possible. The complexities of the surface-runoff system are such that most model components will ultimately rely on empirical relations of some form. However, when these relations are based on the physics of the process, the parameters are more likely to be measurable or readily estimated from climatic and basin characteristics. Physically based parameters provide a larger measure of confidence in their validity and in their transferability to other basins and times.

Improved methodology is needed to provide better measures of the spatial variability of basin characteristics, selected processes, and process parameters, and to incorporate these measures in a meaningful way in a simulation. Existing and proposed technologies for satellite and airborne remote sensing provide measurement tools that need to be explored more fully. Techniques to couple statistical measures of spatial variability with deterministic process simulations also need more development.

The problems of scale need to be considered in the process and parameter- estimation investigations. As noted by Klemes (1983), as one moves from plots to hillslopes to small basins, different sets of physical laws dominate at each major scale. Laws at a larger scale tend to express averages or integrals of those dominant at smaller scales. Likewise, time is a consideration in parameter estimation in that parameters for daily time-step simulations may not be representative for shorter time intervals. The variability and applicability of parameters and process simulations at different spatial and temporal scales needs to be better defined.

Simulation capabilities have generally exceeded available data bases. Data bases are not adequate to test and validate many of the more detailed simulation models, as well as some of the more simplified models. Complete data sets for selected land uses in a variety of climatic and physiographic regions are needed to enable the development and testing of robust process-simulation techniques that are applicable for a considerable range of agricultural and climatic conditions.

The development of improved modeling capabilities needs to be combined with the application of new technologies to resolve problems associated with ease of model use. Interactive programs are needed to assist model developers and users in processing data, initiating model simulations, and analyzing model results using a variety of statistical and graphical techniques. Artificial intelligence and expert systems are tools that could provide some of these capabilities. In addition, standard sets of statistical measures need to be developed to provide a common basis on which to compare the performance of different models and model components and to provide the user with a measure of the confidence limits that can be placed on the simulation results.

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DISCUSSION OF PAPERS PRESENTED IN TECHNICAL SESSION 2, PART 1: SEDIMENT YIELD/RUNOFF MODELS FROM THE MODELER'S PERSPECTIVE

George Hart¹, Presiding
V.P. Rasmussen², Recorder

PAPERS DISCUSSED

Agricultural Nonpoint-Source Runoff and Sediment Yield Water Quality (NPSWQ) Models:
Modeler's Perspective by C.W. Rose, W.T. Dickenson, H. Ghadiri and S.E. Jorgensen

Modeling of Agricultural Nonpoint-Source Surface Runoff and Sediment Yield - A Review from
the Modeler's Perspective by G.H. Leavesley, D.B. Beasley, H.B. Pionke and R.A. Leonard

SPECIFIC QUESTIONS AND COMMENTS

Question: (Audience) What about USLE slope relationships...why didn't we see a range in your data...are we going to get strength data?

Response: (C. Rose, Griffith University, Australia) The majority of the data in my report were from CULTIVATED SOILS. We are currently trying to get more "independent" strength data. In all cases (shown), the shear strength, detachability, and entrainment are about the same.

Question: (G. Hart, Forest Resource Department, Utah State University, Logan, Utah) Snowmelt is often up to 3/4 of the flow in mountainous areas such as Utah...Many models do not address this...Is there any hope of addressing this problem?

Response: (G. Leavesley, USGS, Colorado) Snow melt is addressed in some models. Snowmelt has the greatest impact in detachment. However, many soils outside the USA are a problem because critical data is not available. Another problem is that most weather data (worldwide) is collected by time periods exceeding 12 hours (usually 24 hours) and is not EVENT-related.

Comment: (G. Hart) The ENERGETICS of snowmelt are important and are often overlooked.

Comment: (Audience) Worldwide data (across many regions) is lacking.

Response: (C. Rose) Most of the work presented in this paper is from U.S. civil engineering studies on homogeneous media. We have made computations on wild lands -- with limitations.

Comment: (G. Leavesley) There are two scientists doing work with portable equipment on Mt. St. Helens.

Comment: (Audience) Ephemeral gullies are a problem.

Comment: (Audience) You can calculate what comes off on one field or one river -- but the problem lies in when we expand to two fields, two rivers, or more!

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Response: (D. Beasley, Agricultural Engineering Department, UGA, Georgia) Transport mechanics on the field level are (admittedly) easier. However, I realize the limitations of the USLE.

Comment: (Audience) Periods of less than one year are also a problem with the USLE.

Comment: (Audience) Within a few minutes in a Louisiana storm event, water is falling upon water -- not soil -- and this is a problem!

Response: (D. Beasley) Some workers have studied high-clay soils in situations like this.

Comment: (G. Leavesley) If the transport capacity goes beyond the transport rate, then deposition occurs.

Comment: (C. Rose) Unless we include deposition EXACTLY, we have problems. The only way you can deal with such changes is in the slope. We need experiments involving the size effect on delivery and enrichment ratios.

Comment: (Audience) We need better models for fertilizer management.

Comment: (D. Beasley) GLEAMS, CREAMS, and other models are good efforts on this problem.

Comment: (C. Rose) With all soluble fertilizers, the loss is by leaching.

Comment: (Audience) Downstream impact is the critical problem that we need answers on.

Comment: (D. Beasley) HSPF, etc. does handle pesticides down to channel point of interest.

SUMMARY:

The most vocal concern was that many models do not address the large-scale problems that are of imminent political concern. Most models have been developed with plot-size data and are severely limited when applied to large-scale areas with extreme spatial variability. There are also severe limitations of available data in Third World countries. However, the authors agreed that we are much better off in these areas of concern than we were five years ago. In addition, many researchers are busy extending their "plot-based" models to larger areas and regions of limited data.

THE USE OF SURFACE RUNOFF MODELS FOR WATER QUALITY DECISIONS - A USER'S PERSPECTIVE

George Oliver¹, John Burt², and Rhey Solomon³

ABSTRACT

A wide variety of runoff models is currently being used to address water quality issues from the national to the local field level. The complexity of the surface runoff process and the need to provide information quickly has increased the reliance on these models. To properly utilize a model, the user must clearly understand the goals and objectives of the modeling project, and the capabilities and limitations of the selected model. If the valid uses of runoff models are to increase, improvements are needed in basic model design and structure, support data bases, and user education programs.

INTRODUCTION

Considerable attention has been focused on groundwater during the past decade, but surface water remains an equally important and valuable resource. Maintenance of acceptable levels of surface water quality is crucial for insuring a healthy environment. Due to the complexity of the runoff process and the resulting impacts on water quality, resource professionals increasingly rely on computerized runoff models to assist in the planning and decision-making processes. This paper examines the current and potential uses of surface runoff models in making water quality decisions. Rather than attempt a detailed examination of specific models or uses, this paper presents a general overview from the user's perspective of key aspects shared by almost all approaches to runoff modeling. Detailed discussions of specific model characteristics and procedures for evaluating particular user needs are presented by James et al. (1981), Frere et al. (1982), Larson et al. (1982), Renard et al. (1982), DeCoursey (1985), and Crowder (1987).

USES OF RUNOFF MODELS

Runoff models are currently used at the national, regional, local, and even field level by a wide variety of technicians, researchers, managers and regulators. The most widely used models range from relatively simple empirical models such as the Universal Soil Loss Equation (Wischmeier and Smith 1978) to the more process-oriented models such as WRENNS (Forest Service 1980) and sophisticated simulation models such as ANSWERS (Beasley and Huggins 1981), CREAMS (Knisel 1980) and GLEAMS (Leonard et al. 1986). The selection of a model is dependent on the complexity of the problem, data availability, intended use of the output, and the experience and capability of the modeler.

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National-Scale Assessments

At the national level, the USDA Soil Conservation Service (SCS) has used models to evaluate potential nonpoint sources of pollution. The SCS conducts appraisals based on a statistical sampling of specific points throughout the country. Erosion rates and sediment delivery rates measured for the selected sampling sites are used as inputs to the hydrologic model of Resources for the Future (RRF) to conduct the national appraisal of the erosion rates and land resource conditions for large areas of the United States.

Local-Scale Assessments

At the other end of the use spectrum, runoff models are used by researchers in the agricultural chemical industry and a wide variety of county, state, regional and federal agencies to evaluate the potential for runoff, erosion, and chemical losses from single watersheds or even individual fields. Runoff models are often used by the agricultural chemical industry to determine potential losses with new chemicals, different application rates and techniques, and new use areas (McCall et al. 1987; and Oliver and Eger 1987). Industry researchers have also utilized runoff models to examine available surface water quality data and better determine the reason for chemical runoff losses and develop estimates of predicted patterns of loss based on expected environmental conditions (Gustafson 1987; and McCall et al. 1987).

Educational Uses

The use of models as an educational tool offers tremendous potential benefits for reducing nonpoint source pollution of surface water. The various USDA agencies such as the SCS, Forest Service, Extension Service and Agricultural Research Service (ARS) have been leaders in utilizing models to examine field-scale management programs and to educate the end user (Burt et al. 1984; Knisel 1980; and Wischmeier and Smith 1978). Models are used to assist in determining the effectiveness of various conservation practices and to develop the most appropriate management programs from both environmental and economic perspectives.

Reasons for Modeling

Why a runoff model is used is a key question, and is often difficult for even the modeler to answer. Before an effective modeling approach can be developed, the user must have a clear understanding of the problem and the intended purpose of the output. Typically a model is used to plan, manage or regulate any aspect of a project which involves hydrology, erosion, or sediment and chemical transport, when appropriate field data are not available. Some of the other options to the use of a model would include conducting a field or monitoring study, or relying on estimates based on the judgement of professionals.

Field Studies

The use of field studies to answer runoff questions is often not a practical alternative. Field studies are difficult and costly to conduct, and the researcher usually has little or no control over such key factors as weather conditions. In addition, all field studies (regardless of the level of detail or sophistication) share the same major inherent limitation: field studies demonstrate behavior at one site under a single set of conditions at a particular time. Another major limitation of field research is the time required to conduct the study. Even if the study is successful, the final results are often not available for months or years. During the lengthy study period, the false perception of a problem may have escalated to such a level that scientific reasoning no longer plays a role in the final decision-making process, or a real problem has been allowed to continue for so long that unnecessary environmental damage has occurred.

In comparison to field studies, computer modeling offers the advantage of tremendous savings in time and expense. Once the basic inputs have been obtained and the model calibrated, alternate scenarios can be compared in a matter of days or even minutes, depending on the complexity of the problem. The model allows the user to compare the resulting impacts of changes in any one parameter or combinations of parameters. Similar comparisons are often too costly to conduct under actual use conditions. Also, a model permits the evaluation of 'worst-case' situations. Since the probability of extreme climatic events occurring during the course of any single field study is low, substitution of the desired climatic inputs into a model simulation of field results can be used to estimate the consequences of more extreme conditions.

General Runoff Estimates

Estimates and conclusions developed by individuals or groups of professionals based on their past experience and training are commonly used to answer questions dealing with runoff. Although some type of answer may be available quickly, the decision-making process is hidden and typically only the final answer is made available. Personal bias and erroneous assumptions which may have significantly affected the final answer may not be noted by the audience. In comparison, the development of a modeling scenario provides a documented, traceable, and defensible series of steps leading to the final answer. Although many of the background assumptions made during modeling are still based on the researcher's experience and judgement, the audience is provided with the opportunity to review the process and assign their own level of confidence to the output.

The use of models also increases the potential scope of analyses. Runoff is a highly complex process and a large number of variables must be considered when developing even the simplest of assessments. For example, to estimate the sediment yield and pesticide loss from a typical corn field, a researcher may need to evaluate the influence of such diverse factors as: soil properties, infiltration characteristics, slope, field shape and size, surface condition, tillage practices, crop size and spacing, pesticide dissipation rates and adsorption characteristics, rates and method of pesticide application, crop and residue cover, rainfall rate and duration, and the changes with time of these factors. The input parameters listed only refer to detachment and movement from a point. Transport across the field and further downslope or downstream would significantly increase the number of variables to be considered. A general assessment, formulated by even the most experienced field professional, may not be adequate if the objective is to better quantify the impact of changes in individual factors that are part of more complex interactions or to evaluate the effects of non-typical conditions which may be unfamiliar to the professional.

A runoff model should be used to expand and refine, but not replace the knowledge and experience of professionals. In a runoff model, the ground rules which govern the processes have been established.

Although the role or function of each physical process has been previously defined, total reliance on the expertise of the model developer can lead to serious errors. The end user of any model is ultimately responsible for deciding if the output is reasonable for the given input parameters. The computer only processes the data, and the evaluation of the value and accuracy of the output remains the responsibility of the user.

NEEDED MODEL OUTPUT

The nature of the output needed by the user is a crucial question, but one that is often poorly defined. The type of output required should be dependent on the particular use objectives. For example, when various conservation and management alternatives are compared, accurate simulation of the maximum and minimum values along with the timing of the occurrence of these points may be the most important aspects of the model evaluation. In other situations, such as

determining the ecological impact of sedimentation in a large lake or bay, the total seasonal or long-term loading may be the most critical output.

Regardless of the intended use, no model can be expected to predict the field data exactly. Runoff is a result of some processes which are causal and some which are random. Many of the processes are only partially understood, and the available mathematical simulations represent only general estimates of what is occurring in the field environment. Also, the ability of the model to 'predict' losses from any field situation can be no better than our ability to predict such factors as rainfall, plant growth, or pesticide degradation at that site. An exact match with actual field behavior usually cannot be achieved, but the user should insist that a model simulate the basic trends observed in the field reasonably well. Calibration with available data for a particular site is the best method to improve the predictive capability of a model. If data is not available for the site, results of calibration procedures for similar situations should be examined to provide insights into the type of adjustments which may be needed and to determine the level of confidence the user can place in the output.

CURRENT LIMITATIONS OF SURFACE RUNOFF MODELS

Although computer models offer many potential advantages for obtaining estimates of surface runoff quality, the current use and acceptance of these models remain rather limited, and misuse is not uncommon. Each model may have particular problems, but the following limitations are common to most runoff models and modeling approaches.

Over-Extension of Models

The user often has a poor understanding of the inherent limitations of a particular model. In an attempt to provide an answer in the shortest period of time and with the least amount of effort, many users will rely on basic, empirical models for situations that are too complex to be adequately described by such simplistic models. In some cases, however, misleading output may also result from attempts to use input-intensive models when accurate input data is not available. The detail of the output from these highly sophisticated models may imply a false level of accuracy. The user must also recognize whether the model is appropriate for the particular use situation. For example, runoff models developed for row crop scenarios may not be valid for forestry situations (Nutter et al. 1987). Due to limitations and misapplications, many simple models, such as USLE, are being replaced by new technology with increased sophistication in process representation and wider applicability. (Foster and Lane 1987).

Lack of Appropriate Input Data

The input data needed for calibration and validation are often not available. The time and expense involved in conducting field runoff studies have resulted in a general shortage of data available for modeling. Also, field and laboratory studies are often conducted without consideration of modeling needs, and the resulting data are of only limited value. The lack of suitable input data is often the reason why the more accurate, but input-intensive simulation models are not used.

Runoff Scenario Development

The development of techniques to formulate valid field- or watershed- scale scenarios for runoff modeling has not kept pace with the development of newer models. Many resource professionals, especially among the regulatory agencies and agricultural chemical industry, deal with runoff issues on a nationwide basis and need to develop hypothetical, but realistic scenarios. The inability to

develop more realistic scenarios often results in the use of totally inappropriate data which may invalidate the results of the modeling simulation.

Risk Assessment Procedures

Modeling approaches for risk assessment have generally not been validated or widely accepted. The question of what input conditions should be included needs to be answered. The computer will solve the appropriate equations if the input values allow the calculations to follow the laws of mathematics. The user is typically free to enter almost any value, and this freedom presents the opportunity for misuse. For example, the probable maximum rainfall for a 24-hour period in much of the Cornbelt of the Midwest United States is 28-34 inches over a 10 square mile area (Gilman 1964). Some people might argue that such an extreme event should be used as the basis for a worst-case analysis, but a rainfall of this magnitude would likely invalidate many of the basic assumptions underlying the simulations of field processes. Also, modeling only one consequence of a worst-case event may mislead the audience. Although the actual quantity of sediment, pesticide, and fertilizer lost from a recently treated field would likely be high during a 28-34 inch rainfall, the effects of these losses to society would be small compared to the overall flood damage.

Although many modeling approaches in the areas of both leaching and runoff now utilize a probability function to assist with selection of inputs and interpretation of the output, the probability is most often associated only with the rainfall component (Burt et al. 1984; Carsel et al. 1984; and Oliver and Laskowski 1986). The actual probability of occurrence for the predicted results is also dependent on the probabilities associated with each of the input parameters. For example, when modeling the runoff potential of an applied pesticide, a single value for the dissipation rate is typically used even though the rate will likely vary with time and space across the field. To properly define the probability of the predicted pesticide loss, the probability of the selected dissipation rate occurring across the entire field for the duration of the simulation period should also be considered. Risk assessments produced through model simulations can be greatly improved by the use of the probability concept, but further research is needed to fully quantify this aspect of modeling.

IMPROVEMENTS NEEDED IN RUNOFF MODELS

If the valid uses of runoff models are to increase in the future, improvements in the design, structure, and support programs for these models must continue. James and Burges (1981) have also outlined many of the needs for rainfall-runoff modeling which may be equally important to certain areas of runoff-water quality modeling. Attempts to improve models must first be based on the realization that the majority of model users will not be the model developers. The following list highlights some of the key improvements which would help to standardize approaches and also to increase the effective use of runoff models.

- (1) User-friendly computer code. The code associated with a model should make installation, operation, and understanding as easy as possible. Although the user may actually have a good understanding of the underlying theories, a rigid and poorly designed computer code may prevent the user from following the various calculation pathways. The user must be able to track the decision-making processes through the model to obtain a more complete understanding of the model and to make any adjustments needed to improve the performance of the model for a particular situation. Model developers should also recognize that users will likely have problems running the model, and error messages must be easily understood and helpful.

- (2) Background documentation on the limitations and expected accuracy of the model. Manuals for individual models often provide extensive detail outlining what the model can do, but explaining what the model cannot do is equally important. Internal triggers which issue a warning if the inputs exceed the limits of the model would help to prevent unintentional misuse.
- (3) Input data bases in an appropriate format. Obtaining the appropriate data is probably one of the most common problems encountered by users. Even when the data are available, entering long lists of data for such inputs as daily rainfall may be considered too time-consuming. Development of valid input data bases and proper formatting to allow the data to be accessed by the model without extensive manipulation by the user should be a key consideration of computer program design.
- (4) Recognition of untreated or buffer zones. Most runoff models currently require the assumption that a pesticide treatment occurs over the entire area involved in the runoff process. Generally, banded applications or applications to specific areas or strips within the watershed are simulated by assuming the same amount of pesticide is broadcast over the entire watershed. The effects of the runoff water moving across untreated areas are not included, and the output tends to overpredict losses. The distributed-parameter approach which allows the watershed to be divided into individual and distinct elements (Beasley and Huggins 1981) would be useful for modeling the more complex management scenarios, but also increases the amount of effort required to compile the input files. The capability to easily simulate both treated and untreated areas within the same watershed would greatly increase the usefulness of runoff models for development of farm management plans.
- (5) Leaching and in-stream capabilities. Many of the current runoff models only evaluate surface losses within the field area. To conduct a more complete environmental assessment, both the leaching and downstream fate of the losses must also be considered. The addition of these capabilities to a particular surface runoff model may not be practical or even necessary. The development of software to link the runoff model with widely available leaching, groundwater, and surface water models could be used to enhance the overall usefulness of the model.
- (6) Development of graphics capabilities. Runoff models will often be used as educational and guidance tools. Long lists of printed output often invoke a negative response from the average person, and key messages may be better displayed through graphics. More enthusiasm for the use of models will be generated among users and their audiences if the output can be presented in both an interesting and informative manner.

THE FUTURE OF RUNOFF MODELING

As the capabilities of computers to store and quickly process greater quantities of data continue to increase, more sophisticated surface runoff models will be possible. Along with improvements in model technology, we need to further our research efforts in several associated areas. A more complete understanding of the actual field processes is needed to insure that the simulations are accurate representations of the real world. Better coordination of field studies and modeling projects will increase our understanding of field processes and also increase the availability of data for calibration and validation procedures. Efforts to educate users in the proper utilization of models and interpretation of the output must also be increased. The same type of scientifically-based approaches which are used to guide field and laboratory studies should be developed to improve the validity and effectiveness of modeling assessments.

Runoff models will probably never become so accurate that the output should be used as the sole and final answer to environmental questions. When used properly and in conjunction with other research and planning tools, however, runoff models do have the potential to become key components in our efforts to insure the continued availability of adequate supplies of high-quality surface water.

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USER'S EXPERIENCES AND THE PREDICTIVE POWER OF SEDIMENT YIELD AND SURFACE RUNOFF MODELS

Knut L. Seip¹ and Peter Botterweg²

ABSTRACT

Users' experience with sediment yield/surface runoff models is assessed by discussing i) answers to a survey questionnaire and ii) the authors' own experiences with four models. Results show that simulation models are regarded as useful, and better than regression equations. Few model applications have been used as a basis for government regulations or recommendations. Most users are satisfied with the user-friendliness of the models, and since the 1980's models seem to have improved considerably in this respect. However, many users still hypothesize that increased model complexity increases goodness of fit between calculated and observed data.

INTRODUCTION

This paper gives a summary, not of the achievements of runoff-and erosion modelling, rather it tries to make a synthesis of the "however's". In what respect did the models fail? Why were they not used by those who have a stake in the erosion and water pollution problems? How well are the models supported? Do they require data that are not available? Is documentation incomplete, or so complete that it is not tractable? Can changes be made to the synthesis of the "however's". In what respect did the models fail? Why were they not used by those who have a stake in the erosion and water pollution problems? How well are the models supported? Do they require data that are not available? Is documentation incomplete, or so complete that it is not tractable? Can changes be made to the models, and at what cost? We hope the answers to these questions illuminate possible improvements.

Nonpoint-source pollution contributes significantly to impaired water quality of rivers, lakes, and reservoirs. Humenik et al. (1987) quotes results of a survey which shows that water resources in the USA whose designate use are "impaired or threatened" make up 41% of the total river mileage assessed, 53% of the total lake surface assessed, and 28% of total estuary surface assessed. For Europe as a whole, the numbers may be of the same order of magnitude. In Norway, probably one of the countries with the cleanest water in the world, there are about 400,000 lakes with a total lake area of 16,400 km². Of these lakes, 69 lakes with an area of 1,000 km² (6% of total lake area) have been registered as eutrophic or endangered by eutrophication (Hasle and Kostad 1985). Still, eutrophication is a problem in Norway, partly because the eutrophic lakes are among the lakes with the most intense use for recreation and as drinking water sources.

To investigate and report the use of runoff and erosion models, we have applied two methods. We have a) sent out a survey questionnaire to about 60 researchers and institutions and asked for their experiences, and b) reported our own experiences with the application of several runoff and erosion models.

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THE SURVEY QUESTIONNAIRE

Names and addresses for the statistical survey were obtained from articles used by the authors during their work on runoff modelling, from recent articles listed in "Current Contents" under the heading "runoff" and from a literature survey conducted by Marti (1986). We received about 40 answers, 22 of which could be used directly as a basis for statistics.

We do not know to what degree the answers are representative of model users in general. However we think they give a feeling for the present state of practical use of runoff and erosion models. We have also received reprints. These are listed in the Literature Review section, and the titles give an indication of what is presently being focused on by people applying runoff and erosion models.

The questionnaire is divided into five main sections

- 1) model identification
- 2) problem definition
- 3) data availability
- 4) communication to obtain and distribute information, and
- 5) model implementation.

Questions were often of the multiple-choice type, but with encouragement to make additional comments. The statistics for each section are reported below. The statistics represent applications, not single models, except in a few cases where we cite result explicitly for single models. In some cases we also give support to conclusions by referring to extracts of comments given in the questionnaires.

RESULTS

We asked for the name or acronym of the model and what type of model was used (regression models or simulation models). Most answers identified only one category, but it was pointed out (by Hrisanthou) that in simulation models many relationships and coefficients are calculated by regression equations. The statistics showed that almost all models reported were simulation models (fig. 1). Most of the models were implemented on both mainframe computers and on smaller personal computers as shown in figure 2. Only two models are implemented only on a mainframe computer. Figure 3 shows that about one third of the applications are for continuous runoff situations, a little more for single events and a few for both type of investigations. Some of the models were originally developed to simulate a single event, but were later extended to allow a succession to 'continuous models'. A main property which separates the two types of models is the requirement for data. The models intended for simulation of a whole year or a longer period, the 'continuous' models, seem to require only daily resolution of data (according to comments given in the questionnaires). The result for typical field sizes handled by the models is shown in figure 4. Models are either designed to describe areas around 0.1 km² or have, for practical purposes, no upper limit to field size. The models in the last category often allow for subdivision of the area considered into sub-watersheds, or subfields characterized by uniform soil, vegetation or agricultural practice (half of the models are single-field models and half are multfield models (figure 5). Channel erosion is usually not included in single-field models, and this type of erosion is often quoted as a factor which limits the applicability of the models.

TYPE OF INVESTIGATION

Figure 6 shows the distribution of problems addressed by model users. No problem category is dominating. To identify critical areas for runoff and erosion it is almost necessary to use models

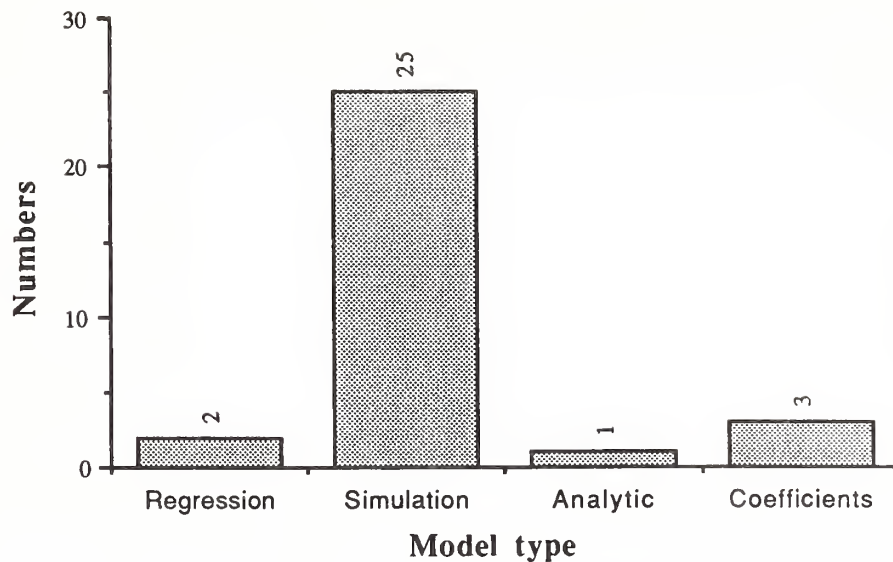


Figure 1.
Types of models. In simulation models, subproblems will often be solved with equations obtained using regression techniques.

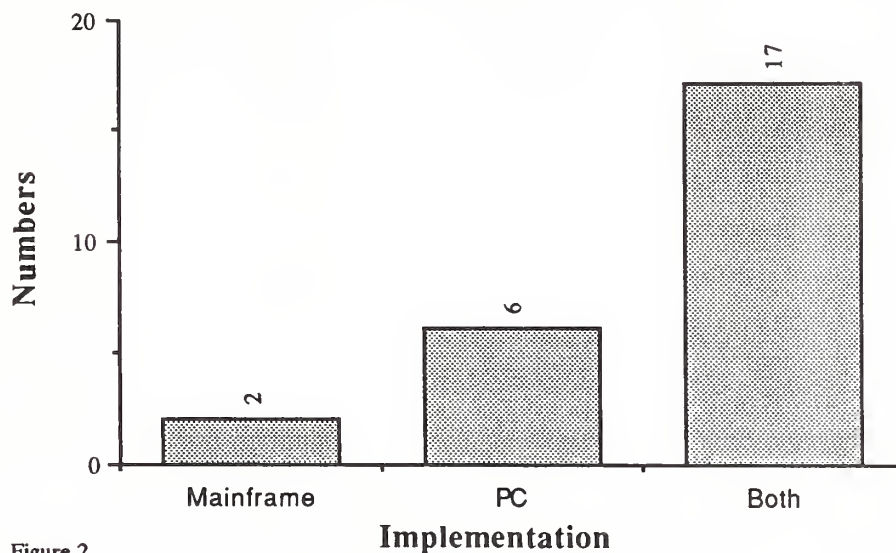


Figure 2.
Implementation of models. Most models are running on both mainframe computers and on PC's.

which allow for the description of several fields. Pollution is, in the questionnaire, identified as pollution of rivers and lakes: however erosion control will, in many cases, also contribute to reduced eutrophication of waterways. In three of the answers to the questionnaire, only erosion control was identified as a problem and not pollution of waters.

Figure 7 shows large government involvement in defining problems, making decisions and being influenced by modeling results. It may be surprising that farmers have been involved to such a small extent (or rather identified by modelers as involved). Farmers are identified as being influenced by the modeling results in 8 cases. This is in contrast to about twice as many cases which include farming practice as a runoff abatement measure. Figure 8 shows how the model results have been used. Only in a few cases have model results been used to give rules or recommendations. In one case it was stated that state and federal agencies required printouts from a model as part of a permit application.

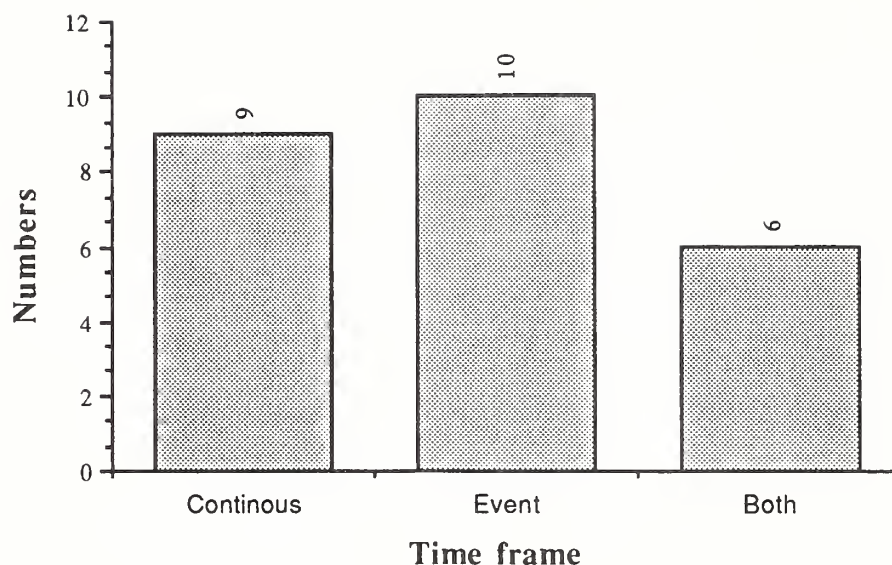


Figure 3.
Time frame of model applications.

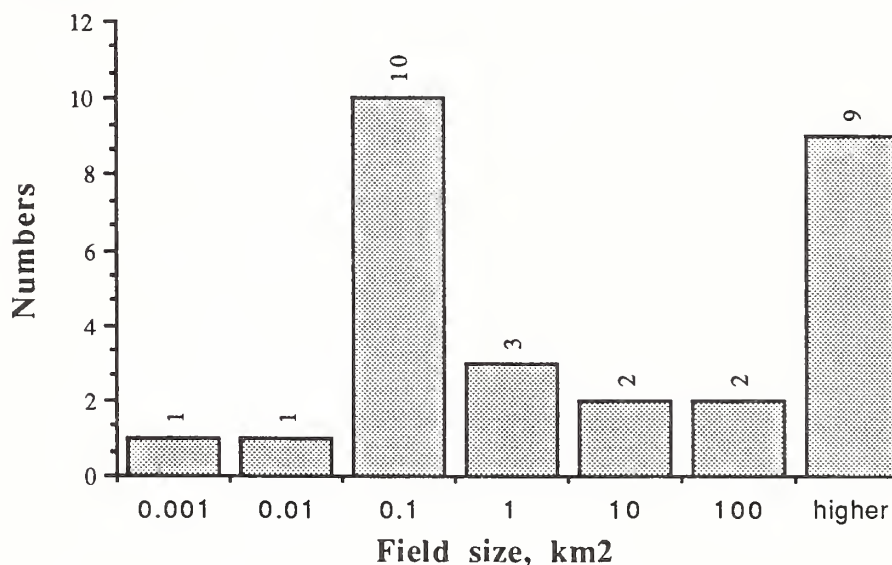


Figure 4.
Field size. The numbers used in the histograms are the upper bracket of values quoted.

DATA AVAILABILITY

We asked for data availability in five categories: climate, topography, soil characteristics, nutrients (nitrogen and phosphorus) and management practice. The list of data was inspired by the data required for the CREAMS model (Knisel 1980), therefore users were asked to fill in missing parameters. We did not define precisely the meaning of "easy" or "difficult" data accessibility. We assumed that data like precipitation and temperature would be about uniformly available and thus set the scale. The results in figure 9 show that nutrients and soil characteristics have been most difficult to prepare, but topography and climate was not as easy to derive as we expected. Figure 10 shows results for the assessment of availability of specific data types within the five groups. Soil particle distribution and phosphorus data are reported to be the most difficult to obtain. Among the topographic features which are most difficult to obtain are stream slopes and width. It is also difficult to select subareas which have uniform characteristics.

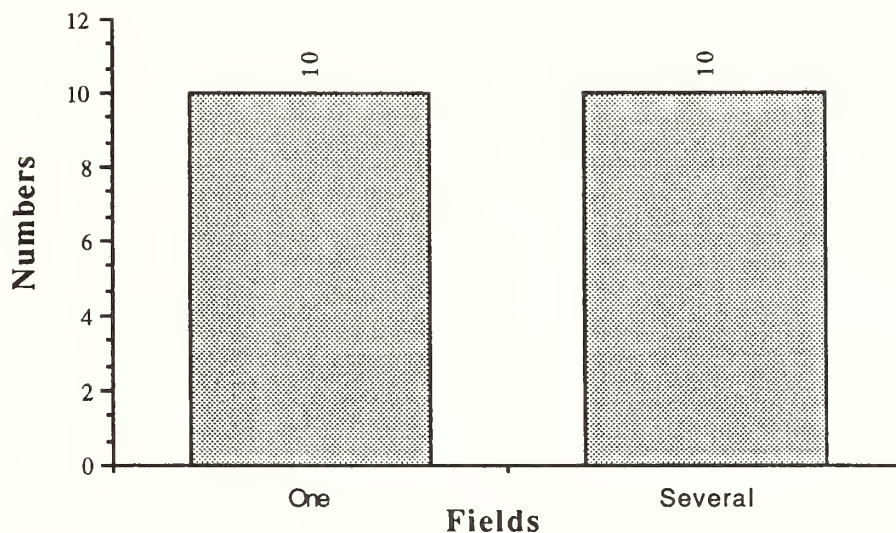


Figure 5.
Space frame of model applications. Models which describe only one field usually only treat overland flow and not channel flow.

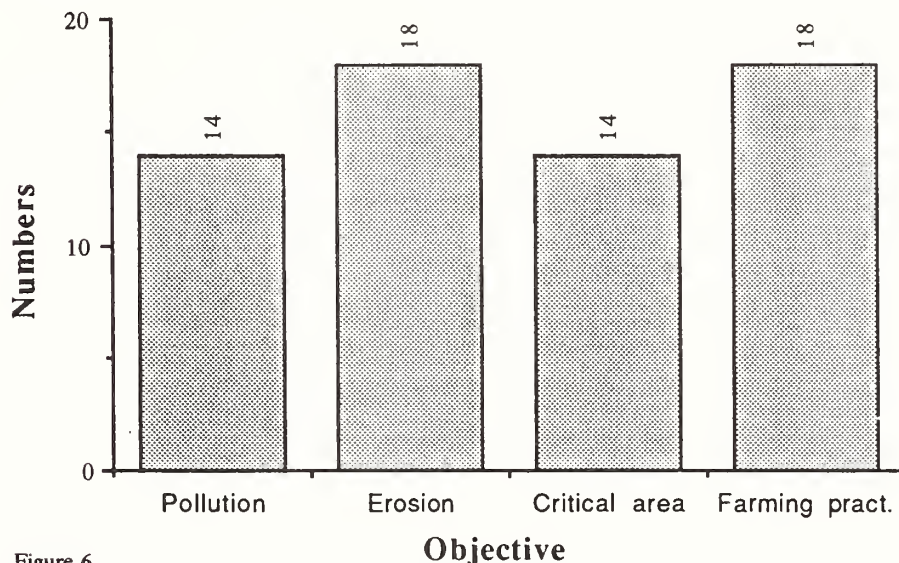


Figure 6.
Objectives. Identification of critical areas requiring a multi-field model.

Figure 11 compares how one model developer rates the accessibility of data for his model compared to three users of this model. It is seen that the users rate data more difficult to obtain than does the modeler. However, the modeler in this particular case has published comprehensive model documentation, including a user's manual giving very thorough instructions on how to obtain the data.

SOURCES OF INPUT DATA AND COMMUNICATION OF RESULTS

Where do model users obtain their data, and how do they communicate their results? Figure 12a shows that literature and agricultural advisers are the principal sources of information "No. 1" indicates that this source has been listed as the most important; "Weighted" indicates the relative importance of the source. This is, for each source, calculated by weighting and summing its score

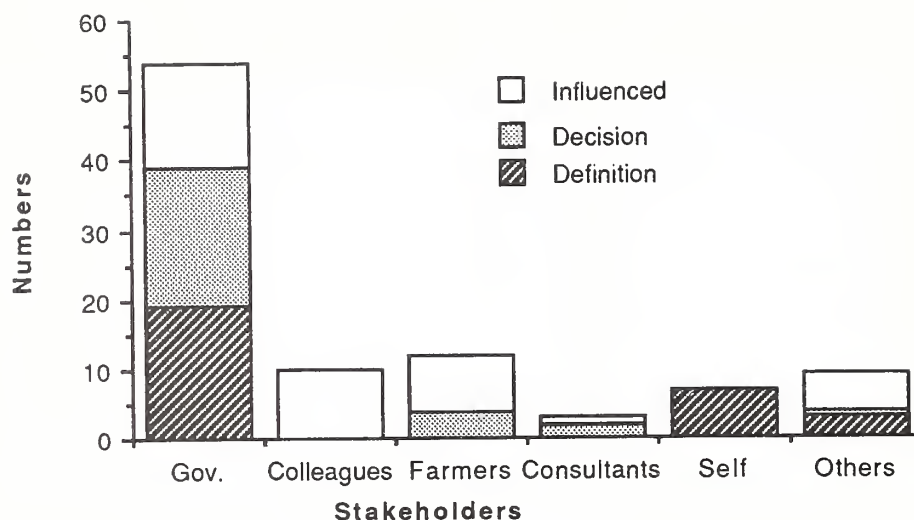


Figure 7.
Stakeholder in model use. Divided into those i) defining the problem ii) making decisions based on modeling results and iii) being influenced by the results.

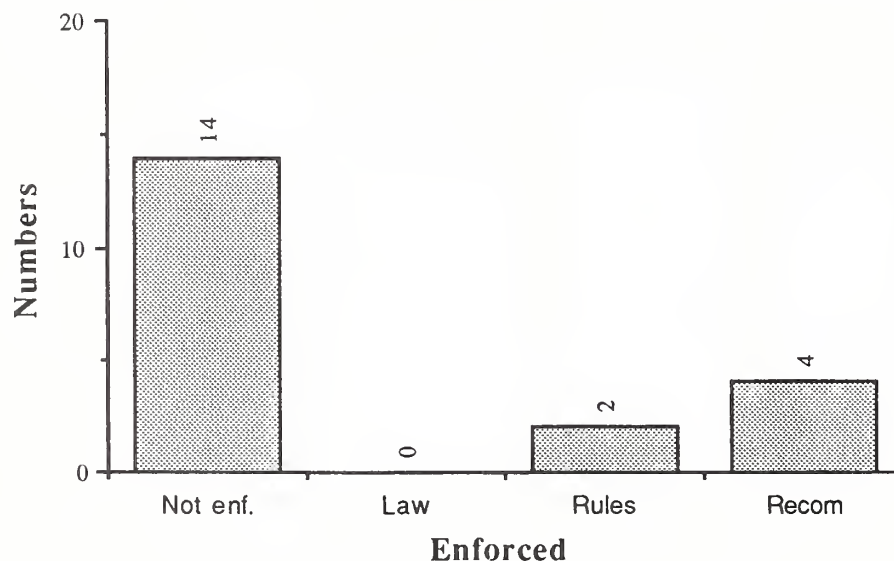


Figure 8.
Use of model results.

as number one, two and three in importance. Figure 12b shows that information is mostly obtained in written format.

Many model users state that the models have not been used for any practical purpose. In cases where they have been used, oral communication to decision-makers dominates (fig. 13a). It may be surprising that interactive communication has been used as much as indicated. The degree of professionalism desired or required for model use is rather high as shown in figure 13b. Farmers are never indicated as a primary user, but they are indicated as a possible user in some cases.

IMPLEMENTATION

Figure 14a shows that most users are fairly satisfied with the user friendliness of the models, support by model developer, documentation and the possibilities for making changes in the model.

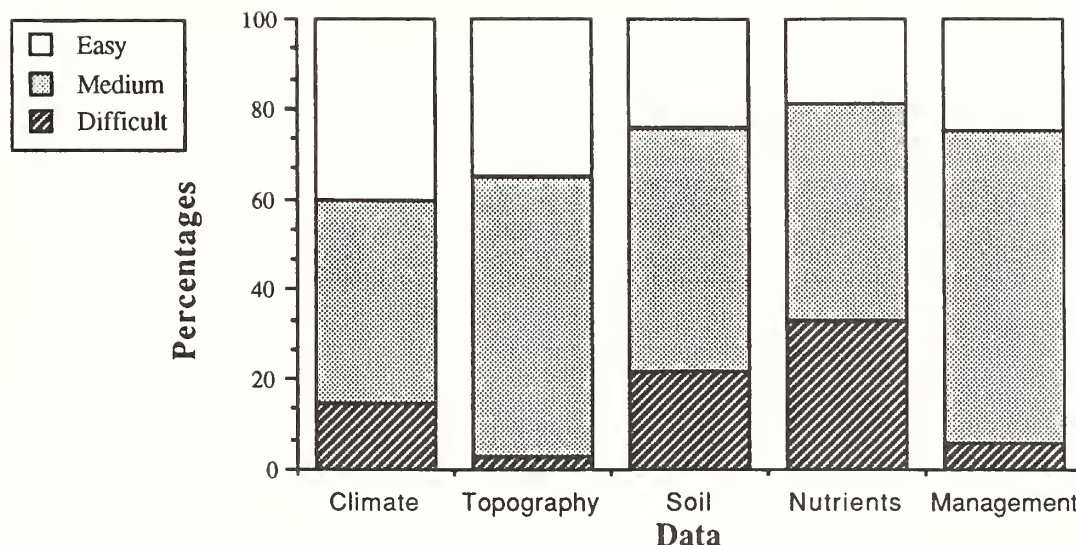


Figure 9.
Data availability (relative scale).

However, many users also point out ease of use as a primary goal for improvements (fig. 14b). Few users actually made changes in the programs (5 vs. 11) and in nearly all cases the modelers were available for comments (figure 15). The figure also shows that all respondents said that the models were useful and better than regression equations. However, several users preferred to make this statement in the comment section of the questionnaire. No particular use dominated the list of answers - simulation models seem to be useful for all reasonable applications within the field of runoff and erosion studies.

OUR EXPERIENCES WITH MODELS

In 1985 the Norwegian Government in cooperation with the Agricultural Research Council of Norway initiated a research and "action" program to reduce nonpoint-source pollution. Included in the program was an experimental part examining the effects of changing agricultural practice in four regions of Norway (Aaker¹). A research project was also initiated with the objective of making available for Norwegian agricultural conditions a mathematical model which could:

1. Quantify the effect of changes in agricultural management on erosion and losses of nutrients and pesticides to open waters;
2. Identify subareas in a watershed which contribute most to the nutrient load on open waters; and
3. Be used by local agricultural and environmental service authorities.

The presentation below gives a survey of the authors' experiences with three models developed elsewhere, and one model developed by one of the authors (Seip and coworkers). The presentation is arranged according to the model examined, but the authors have examined the models separately. When references are made to comparisons between simulated results and observations, this refers to work done by Seip and co-workers.

¹Aaker, Reidun. The "action plan for Norwegian Agricultural Pollution Control. GEFO/Norwegian Agricultural University, ÅS, Norway (in Norwegian).

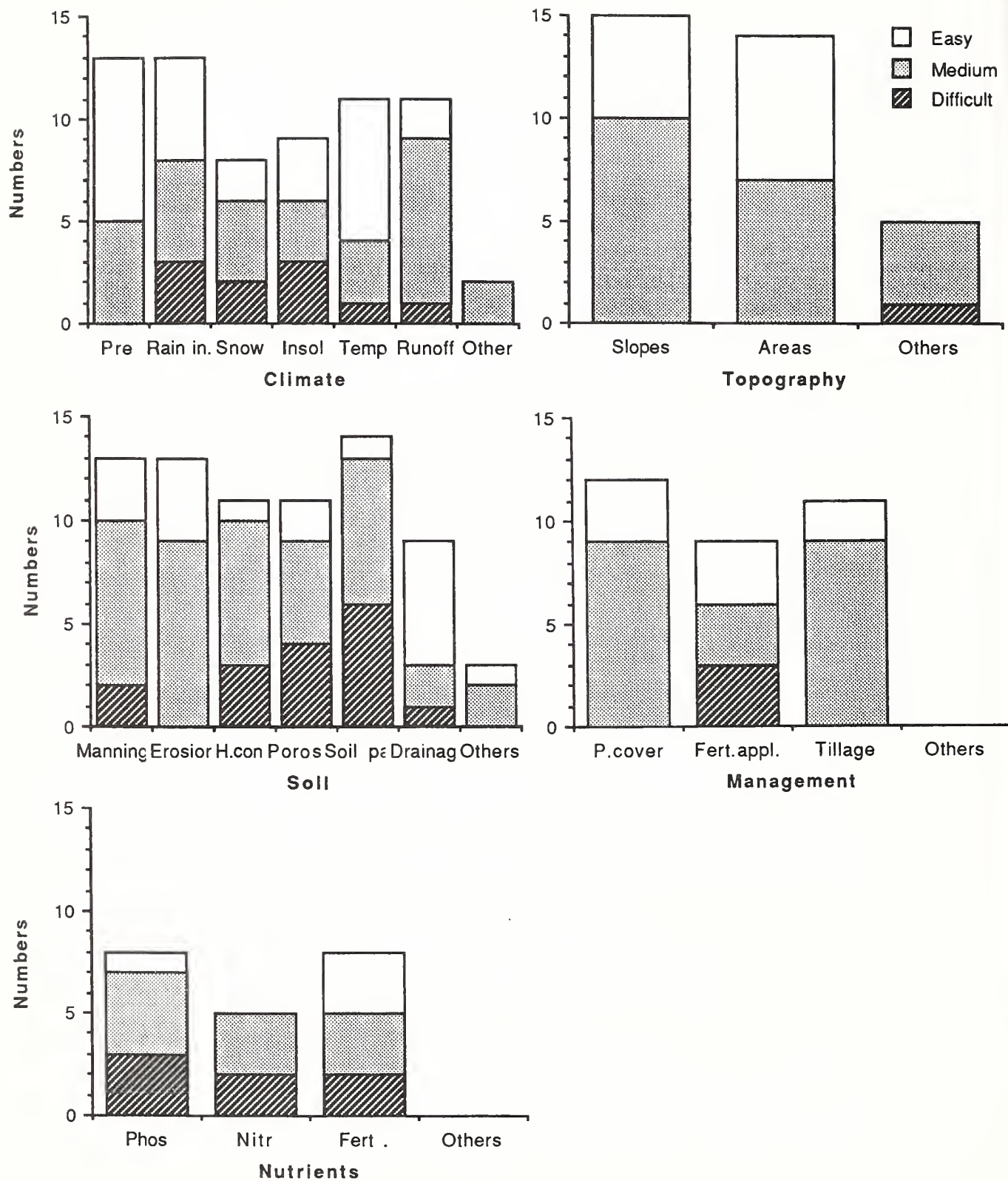


Figure 10.
Availability of data required for model application.

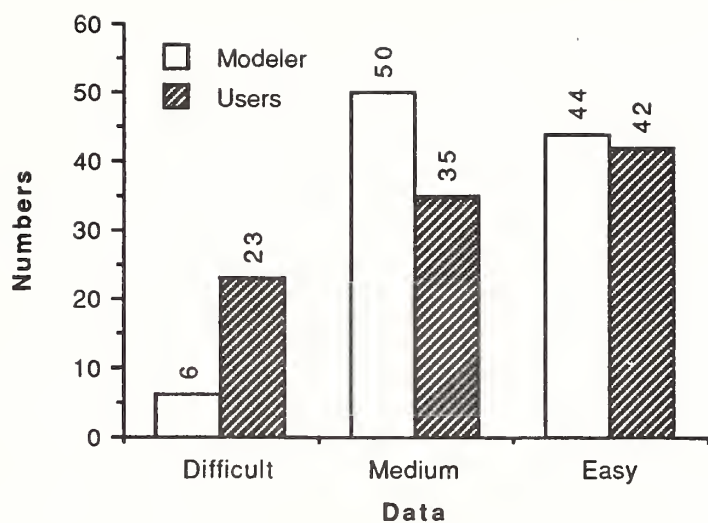


Figure 11.
Difference in assessment of availability between model developer (Knisel) and model users (N=3).

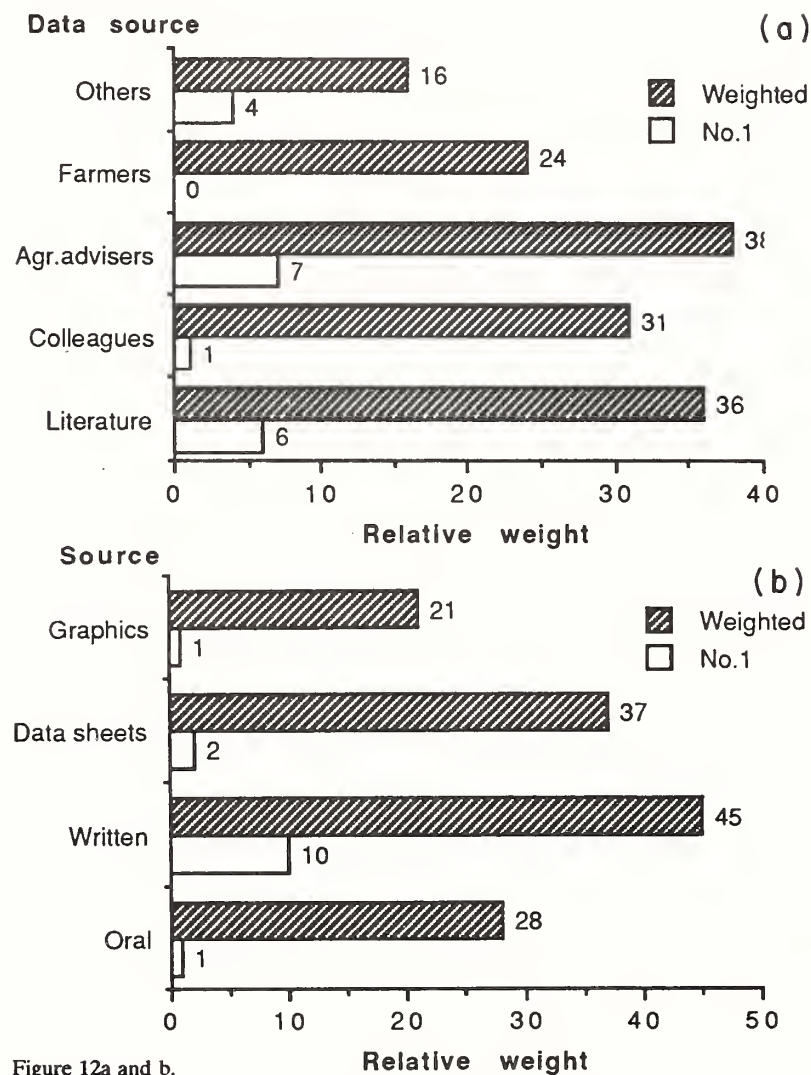


Figure 12a and b.
Data acquisition and communication of results. a) Sources b) Mode of communication.

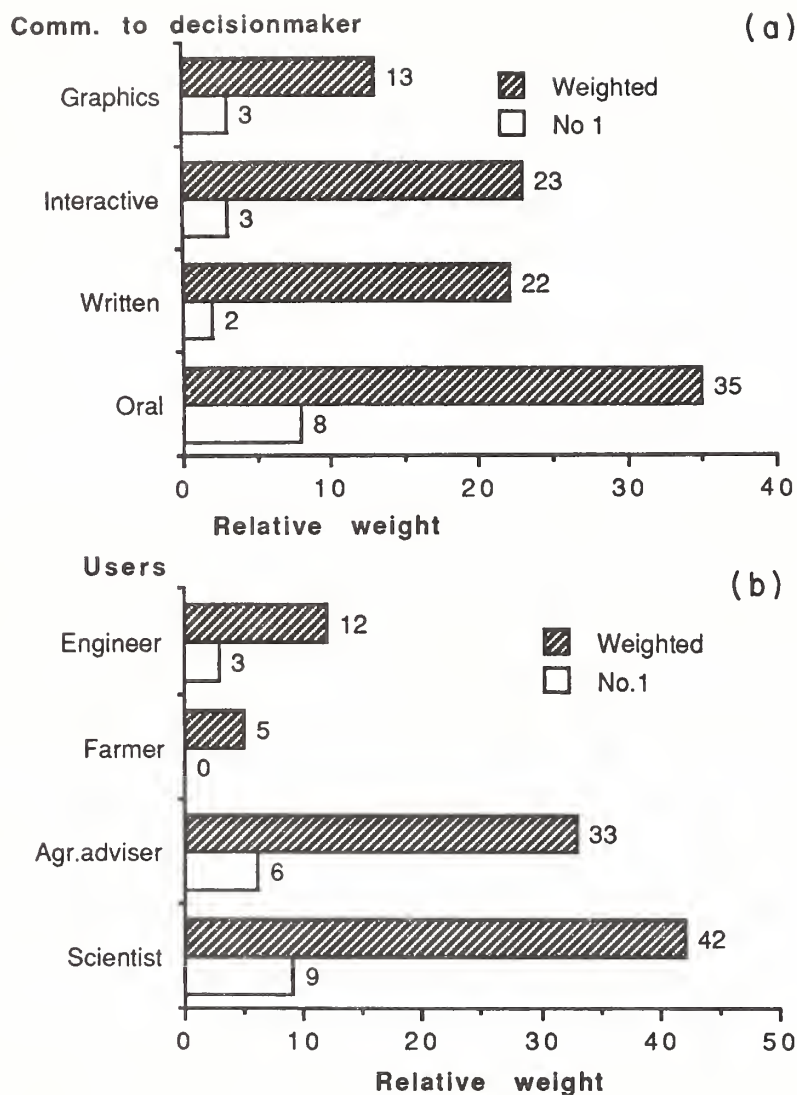


Figure 13a and b.
Model use and degree of professionalism required, a) Communication to decision maker, b) Professionalism of model user.

AREA DESCRIPTION

We have applied both the CREAMS model (Knisel 1980) and the GAMES model (Cook et al. 1984) to Årungen watershed in the eastern part of Norway. The watershed is situated close the Norwegian Agricultural University and is therefore well studied (Grøterud and Rosland 1982). The watershed has an area of 7.9km². The largest part (68%) is in wheat and rye crops. Annual precipitation is 780 mm, with lowest and highest monthly averages of 27 mm in March and 96 mm in August. The average temperature is 5.5°C with the coldest monthly temperature of -5.2°C in January and the warmest, 16.8°C in July.

THE CREAMS APPLICATION

The CREAMS model is described by Knisel (1980). The model consists of three separate modules which treat soil hydrology, soil erosion, and nutrient and pesticide losses. The hydrology module

calculates runoff with the Curve Number Method (USDA 1972) combined with evapotranspiration and percolation. The erosion component estimates erosion and deposition by sediment size traditions along the watershed. Chemical losses are calculated as a sum of losses by runoff, erosion and leaching. At the time of our application we only had the first version of the manual available. Later a second, more user-friendly, version has become available. The user's guide was well organized, but the description of the individual parameters were often unclear, and parameters often were difficult to obtain. The U.S. terminology caused difficulties when European nomenclature and units had to be converted. The model was applied in the sequence: hydrology, erosion and chemicals to the Årungen watershed. The model ran on our NORD computer without any problems, however we had to make a few changes. Of incidental interest is that the sine equation describing the monthly solar radiation was not able to reproduce the sharp decline in light intensity during wintertime found in Nordic countries. We also found that changes had to be made to the snow-melting routine (Kalgraf 1984). Simulation results and observations were compared using equation 1 (Loague and Freeze, 1985).

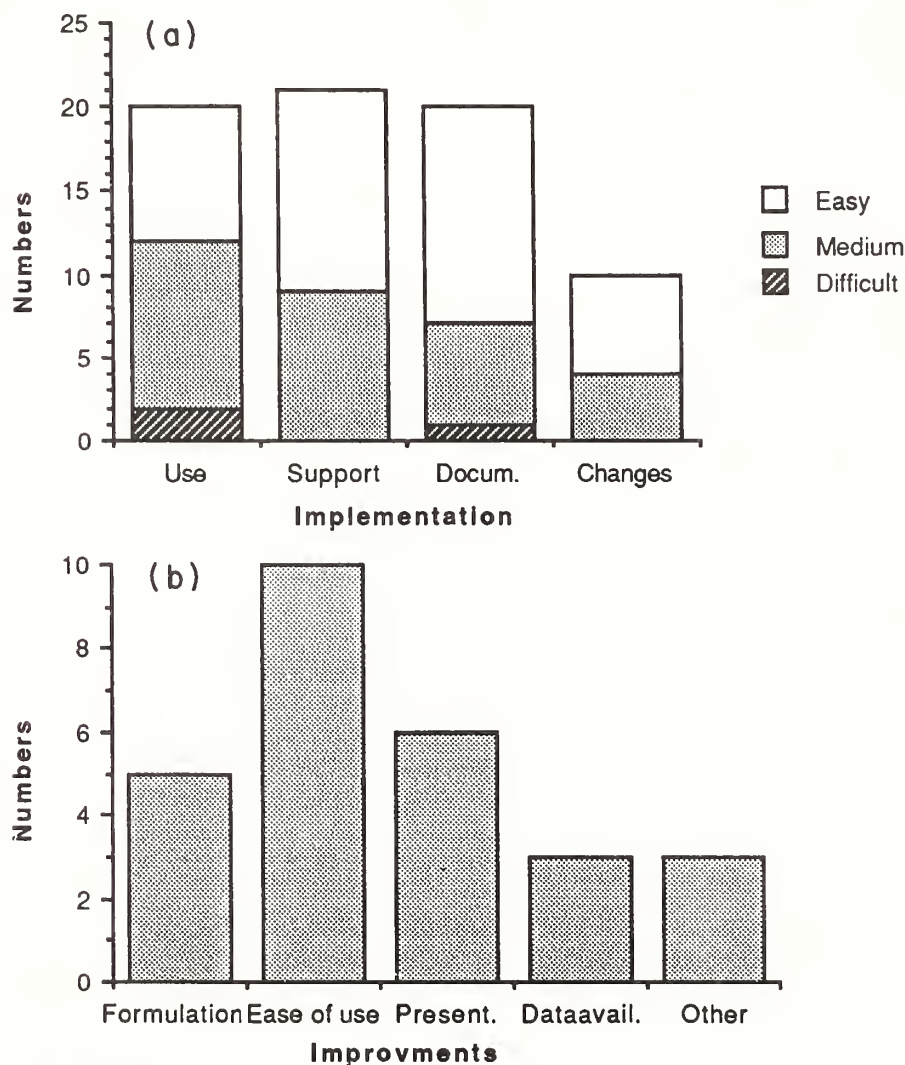


Figure 14a and b.
Model implementation a) status b) improvements

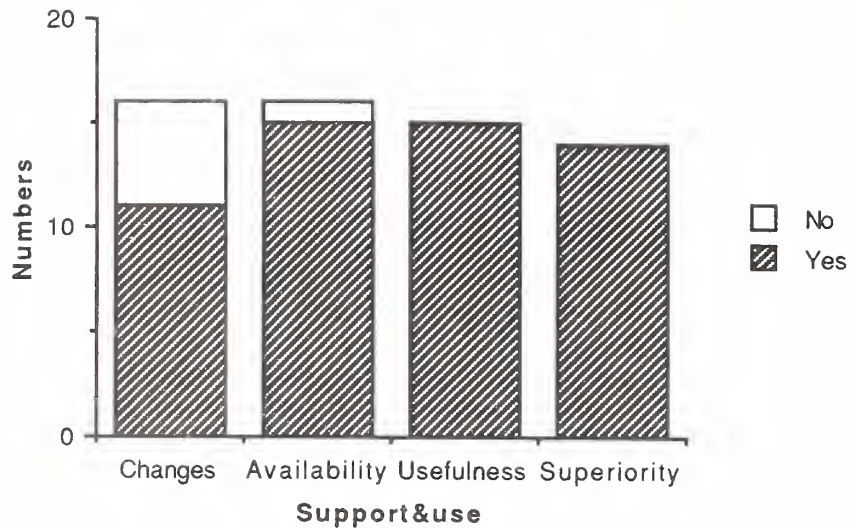


Figure 15
Usefulness of models.

$$E_f = E_o^2 - E^2 / E_o^2 \quad [1]$$

where E_o^2 = the sum of squares of the difference between calculated value and the average value over the verification period $Q_i - Q_a$

E^2 = the sum of squares of difference between calculated and observed value $Q_i - Q_{obs}$.

If $Q_i = Q_{obs}$ then $E_f = 1.0$. If $Q_i = Q_{av}$ then $E_f = 0.0$. E_f may also have lower values indicating that the model gives no improvement in prediction over using the observed overall average value.

The CREAMS model was used for the years 1979-82. Although the Årungen watershed is much greater than the field size recommended for the CREAMS model, we wanted to examine if the model could be used for a whole watershed. Secondly, we wanted to compare the performance of this model with the performance of a multifield model like GAMES, described below. We calibrated one parameter, the contour factor, with data from the year 1979.

The result for runoff (monthly averages) showed E_f values of 0.52, 0.80, 0.52, and 0.04 for the years 1979-1982 respectively. The average for the whole period was 0.36. When we presented the results, especially for the year 1982, people responsible for the runoff measurements were more inclined to assume that the runoff observations were wrong than to criticize the model. This indicates that the models may act as an instrument for validating observations. The results for annual sediment yield were fair, being within 30% of the observed values. Other reports on the use of the CREAMS model can be found in Svetlosanov and Knisel (1982).

THE GAMES APPLICATION

The GAMES model is described in Cook et al. (1984) and Rosseau et al. (1987). the model is based on the Universal Soil Loss Equation (USLE, USDA 1978). The model treats the watershed as a sum of subfields. The fields (cells) can be of any shape. Each field is supposed to be uniform in all of the soil and farming parameters used in the USLE, and erosion material from one field can enter only one of the other fields. The output of the model is a list of subfields and their contribution to the sediment yield (tonnes/ha) or phosphorus yield (kg/ha) at the terminal point of

the watershed. We found the model description and the user's manual clear and instructive. The rainfall factor (R) and the soil erodibility factor (K) were most difficult to estimate. For our model application the watershed was divided into 197 subareas. Subdivision was done manually, and required professional judgement. The result showed that for this watershed most of the eroded material was moved downslope but not off the watershed. During a period of one year, only 7% of the eroded material ended up in the waterways. When we aggregated cells to conform to two subwatersheds where phosphorus (P) observations were done, the model gave 1.69 and 1.94 tonnes P/ha/yr for the two areas. The corresponding observed values were 1.76 and 1.23 tonnes P/ha/yr, ie. the areal with lowest observed P yield is the area with the highest calculated yield. It was indicated by Sannes and Seip (1985) that the reason was that some cells gave very high yields in the model, and that the data for these cells may have been in error. It is interesting to note that Sannes, after having prepared the data for 197 cells was able to predict "manually" with one exception which ten cells the model would predict as giving the highest yield.

THE SOIL MODEL

The SOIL model (Jansson 1980) is a physically based hydrology model for a soil column. We decided to substitute the SOIL model for the hydrology module of CREAMS. The SOIL model requires 162 input parameters, most of these are easily available. From the output of the SOIL model it has been possible to create a file which substitutes for the hydrological output file in CREAMS. It is expected that the SOIL/CREAMS model will give better estimates of runoff, percolation and evapotranspiration than the CREAMS model alone, because of the improved routines for frost and soil cover. However, work on this comparison is not yet finished.

THE SI MODEL

This model is an attempt to merge the multifield concept from the GAMES model with some of the solutions to runoff modeling and erosion from CREAMS. In addition, the model has been developed with a friendly interface to the user. All data input occurs via a menu communication screen. Default values exist for all data. If only default values are used the default value set acts as a test set. On a next higher level, key data can be given which assist the user in selecting correct data. For example, a description is given of several types of field textures and channel tubes (see Chow 1959) and by selecting one description the model proposes a value for Manning's n. To facilitate the retrieval of climatic data the user is asked for the geographical coordinates of the field. Then the average values for light intensity and temperature at the selected latitude are chosen as default values. At the final level of data input the user is asked for technical terms like Manning's n or asked to accept the proposed value. It is our intention that the model shall be used by the same people who use other agricultural models, for example models for fertilizer use. The model has been used preliminarily for two watersheds. It seems to give good results for typical East-Norwegian agricultural areas, however we had difficulties in determining appropriate input parameters for a watershed on the west coast, where manure handling is a great problem.

DISCUSSION

USER FRIENDLINESS

There seems to be a tendency to develop models which can be used on a personal computer. We believe that the idea is that the models shall be useful also for local authorities (and farmers?). The user friendliness of the models is probably not very high. One model developer stated that his model was the best supported and best documented model available, and sent us 3 kg of

documentation, including more than 600 figures in an appendix. In the accompanying questionnaire he also defined "moderate ease of use" for the models as 3-6 months familiarization and a high degree of computer literacy. I would guess, and hope, that most answers to the question of model implementation reflect less strict requirements. In the near future the technical use of the models will be facilitated by adopting modern techniques for machine user interaction like windowing techniques, draw-down menus, guidance by tree structures, etc. We also believe that modern knowledge based systems techniques (KBS) will ease the acquisition and retrieval of information. Since 1980 there seems to be a clear trend toward more user friendly computer programs (fig. 16).

DATA ACQUISITION

Some of the users note that data were easy to obtain because they could be read from a table accompanying the user's manual. To highlight this statement: referring to the CREAMS model (Knisel 1980 p. 44); it is easy to derive maximum rain intensity or a rain index from daily precipitation data, because the model contains a regression equation describing the relationship. However the coefficient of determination $R=0.56$ is not very high (cf. also Kinnell 1987). The construction of the model will often reflect the degree of confidence in the data which the model developer has determined is necessary. However subsequent model applications may identify certain parameters as more critical than others for particular situations. For example: DiSilvo (1983) emphasizes "slide and debris flow" as more important than "surface erosion" for sediment yield calculations in Alpine watersheds. Therefore in the future we can envisage models in which the problem is first identified, and the model thereafter responds by giving a priority parameter list. Data "complexity" (expressing the degree of effort to obtain data for the model) is shown schematically in figure 17. If our assessment of the complexity is correct, there is a trend toward decreasing data complexity in recent models.

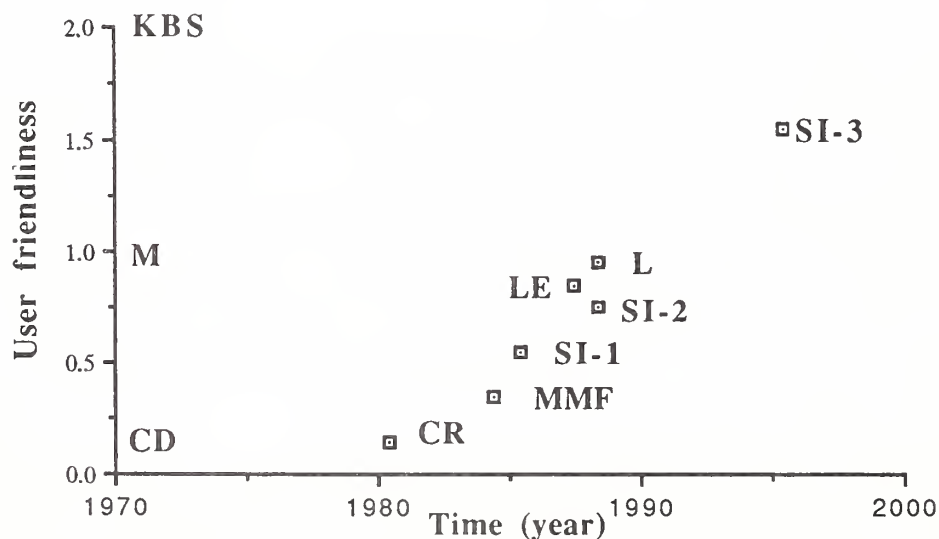


Figure 16.

Development of user friendliness from 1970 to 1990. The ordinate has a qualitative scale: "0" corresponds to techniques such as loading information from card decks, "1" corresponds to the use of MacIntosh techniques, and "2" corresponds to knowledge-based systems (KBS) support techniques. CR=Knisel (1980), L=Leonard et al. (1988), MMF=Morgan and Finney (1984), SI (1-3)=Seip and Kalgraf (1987) LE=Lee and Camacho (1987).

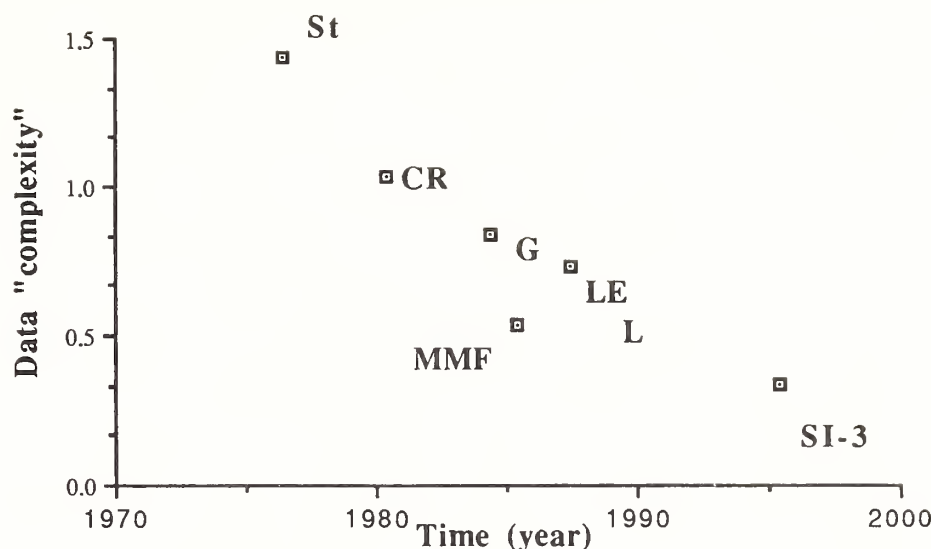


Figure 17.

Data "complexity" required for models from 1970 to 1990. The ordinate has a qualitative scale. "0" corresponds to data on the level of soil group classification data, "0.5" corresponds to USLE data requirement, "1.0" corresponds to Manning's n . St=Stanford model, CR=Knisel (1980), L=Leonard et al. (1988), G=Cook et al. (1984), MMF=Morgan and Finney (1984), SI=Seip and Kalgraf (1987), LE=Lee and Camacho (1987).

MODEL FORMULATIONS

Model formulations sometimes reflect the state of the art in understanding the physical process in runoff and erosion. Often complex formulations also require very good data availability. There are indications that for practical purposes simple models may perform as well as complicated models (fig. 18). Braun and Lang (1986) show for snowmelt that five different methods with increasing complexity for calculating snowmelting runoff gave about the same results for 4 basins (79-1696 km²). The simplest model, the temperature index method of Bergström (1976) may therefore be chosen, at least for large area modeling.

Another example where simplification may be appropriate is in formulations of detachment and transport of eroded material. Moragan et al. (1986 p. 156) and Edwards and Burney (1987) indicate that erosion in most cases is limited by transport capacity. Thus complex formulations of splash detachment (Bradford et al. 1987 a,b Wright 1987, Kinnell 1987) may be of secondary importance. These two results are somewhat in contrast to responses in the questionnaires, where the authors often quote improved modeling formulations as a solution to poor correspondence with observations. However, if more complex formulations are required, our own experience indicates that at least for one model (CREAMS) it was relatively easy to substitute one program module with another sub model. Experiences with the SI model indicate (Seip and Kalgraf 1988) that subdivision of watersheds probably is the most important factor in improving predictions. Cf. also Braun and Lang (1986).

COMPARISON OF SIMULATION RESULTS AND OBSERVATIONS

Several techniques have been proposed to compare simulation results and observations. Equation 1 has been used by several authors; Braun and Lang (1986) find that the criterion reflects fairly well the general conclusions of model performance based on visual inspection. Morgan and Finney

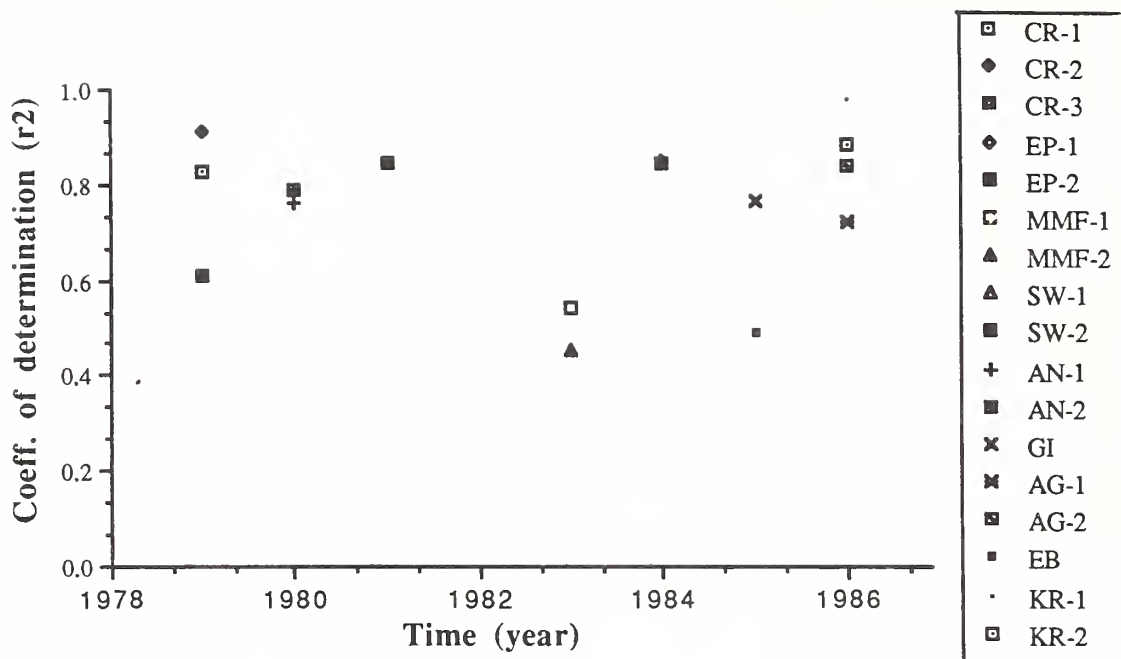


Figure 18.

Goodness of fit between simulated and observed results obtained with increasingly complex models. Goodness of fit is measured by model efficiency, Ef (see eq. 1 in text), B&L=Braun and Lang (1987) on complex snowmelt), GØ=Gørgens (1983 on daily vs. hourly input), L&F=Loague and Freeze (1985 on runoff modeling techniques, however, some errors may have occurred in the observed data, Woolhiser, personal communication).

(1986) and Morgan and Morgan (1981) argue that linear regression is unsatisfactory both for comparing simulation results to observations and for the identification of constants and exponents in the model. For comparisons, Morgan and Finney (1986) use reduced major axis lines. However, as with linear regressions, outliers tend to dominate. They therefore propose an alternative evaluation for erosion calculations which contains a threshold value at low numerical values and a ratio criteria elsewhere. We think that none of the methods quoted above are quite satisfactory, and believe that better methods should be developed. Also "Ocam's razor" should be applied to all digits of constants and exponents.

Developments in model performance from 1980 to 1990 is assessed by plotting the coefficient of determination (R^2) of linear regressions between simulated and observed results as a function of time. Figure 19 shows that there is no trend toward better performance. This probably reflects more the absence of systematic model assessment than a significant lack in model improvement. Better assessments could be made if models were easier to use, and therefore used more often. And if they automatically could produce a final report giving key data for the fields studied, results obtained, and a measure of the goodness of fit with observations. Maybe they could even print the address of the model development center a "postage paid" mark.

We found no reports on failures in predicting the effect of changes in management practice, but we did not find many positive conformations either. It may be that good data sets for the validation of model results are lacking. Our own experiences show that it is very hard to find significant differences in runoff or erosion between fields being subjected to different, but realistic,

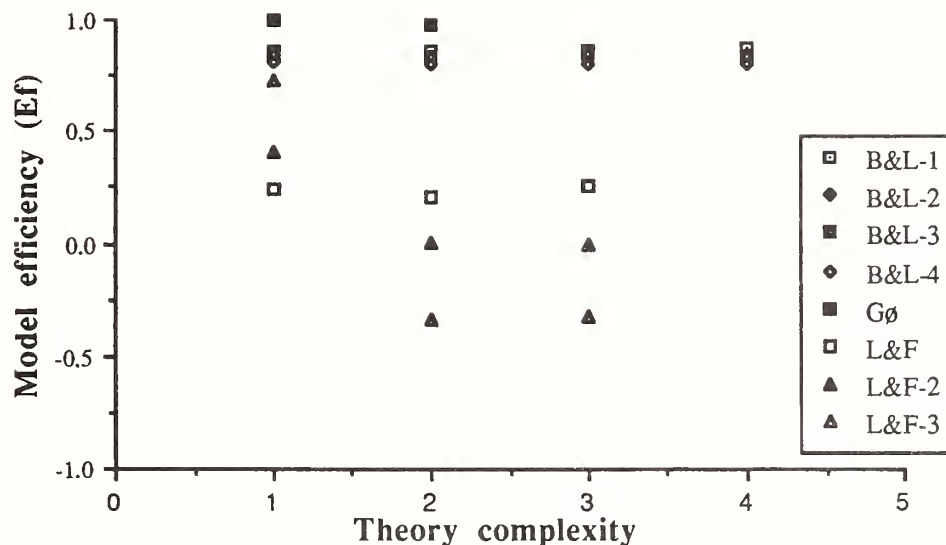


Figure 19.
Goodness of fit between simulated and observed results obtained with models from 1980 to 1986. Results for the applications of the models CR=CREAMS, SW=SWRRB, EP=EPIC, AN=ANSWERS, and AG=AGNPS are from Bingner et al. 1987. MMF=Morgan and Finney (1984), EB=Ebise and Goda (1985), GI=Gilley et al. (1985), KR=Khanbilvardi and Rogowski (1986b).

management practices. Differences in manure handling may be an exception². Another important feature in comparisons of models is the use of "average" or "extreme" meteorological time series. We propose that ten standard time series be developed for precipitation and temperature characterizing different agricultural regions of the earth and that these be published so that they can be used by modelers, and model users.

APPLICATION OF MODELING RESULTS

A model is often developed and calibrated on the basis of a geographically limited set of data. CREAMS was, for example, developed for areas typical of the United States. This will have an effect both on model formulations and on parameter choices. When we used the model for Norwegian conditions, we had to change some of the formulations, and we had to include a better formulation of manure handling. A series of factors (Barrington et al. 1987 a,b) were not described, and we believed that some of these might be important for agricultural runoff models applied to certain areas of Norway where manure handling is a great problem. In other instances, other factors might be important. To handle the problems of model applicability, we believe that knowledge based techniques can be a valuable tool in preparing the model for certain case studies (Seip and Ibrenkk 1987). In the parameter input mode the model may ask questions which identify the case studied and determine if the parameter is appropriate for the situation, or what type of errors the user has to accept.

ACCEPTING MODELING RESULTS

Response from the questionnaire indicated that model results for runoff and erosion were accepted, at least compared to results obtained with runoff coefficients and the USLE. However,

²(Aaker 1988 GEFO, Ås, Norway in prep.)

farmers' interests are not considered to a high degree. For U.S. circumstances this seems to correspond to results reported by Parent and Lovejoy (1982) that farmers (60%) think the federal government should play an important role, in terms of both technical and financial assistance. We do not know the attitude in Europe, but we believe it will be a great advantage if model use could be made user friendly for the farmers.

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DISCUSSION OF PAPERS PRESENTED IN TECHNICAL SESSION 2, PART 2: SEDIMENT YIELD/SURFACE RUNOFF MODELS FROM THE USER'S PERSPECTIVE

George Hart¹, Presiding
V.P. Rasmussen², Recorder

PAPERS DISCUSSED

The Use of Surface Runoff Models for Water Quality Decisions - a User's Perspective, by G. Oliver, J. Burt and R. Solomon

User's Experiences and the Predictive Power of Sediment Yield and Surface Runoff Models by K.L. Seip and P. Botterweg

SPECIFIC QUESTIONS AND COMMENTS

Comment: (Audience) In many cases, the pesticide routines are added to the models as an afterthought...and surface waters are surveyed 1/10 of the rate needed by the best models. This means many regulations are written WITH INADEQUATE DATA and the companies are lacking data to adequately plan and prevent problems.

Response: (G. Oliver, Dow Chemical Company, Michigan) Yes, it is tacked on as an afterthought. It is a very REAL problem.

Question: (Audience) Is a coefficient of determination of 0.8 acceptable as a measure of model accuracy?

Response: (K. Seip, Center for Industrial Research, Norway) I am always skeptical, but it is good when you consider the reliability of the input data.

Question: (Audience) What about incorporating Expert Systems Databases into these models?

Response: (G. Oliver) This will help, but they (Expert Systems) do not always (correctly) determine what you want. Some (incorrectly) allowed cotton to grow in Maine because the user plugged-in ME as the state identifier.

Comment: (K. Seip) AI and Expert Systems are a good thing when they aid you in making the input and boundary condition decisions.

Comment: (Audience) I am concerned about Expert Systems vs. reliability of user. Somehow, we need a "driver's license."

Comment: (G. Hart, Forest Research Department, Utah State University, Logan, Utah) You really don't need a license to drive a car! (...only to drive it LEGALLY!)

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Comment: (Audience) In Germany only a government agency would use models to set regulations.

Comment: (K. Seip) However, even advisors need models that are easier to use.

Comment: (Audience) Abstractions of models are often used by farmers rather than the model itself.

Question: (G. Hart) What about problems of scale?

Response: (G. Oliver) This is a BIG problem because you increase variability. What input do you need at a larger scale?

Comment: (K. Seip) I agree!

Question: (A. Lumb, USGS, Reston, Virginia) Another problem is just WHO makes a model user-friendly? Universities don't reward! Agencies can't do it!

Response: (G. Oliver) It is hard for the developer to step back and make it user friendly! Someone else, often, needs to help.

Comment: (V. Rasmussen, Soil and Water Conservation Research, Utah State University, Logan, Utah) The Association of Agricultural Computing Companies has petitioned Land-Grant Universities in the United States to allow "joint ventures" where commercial concerns take University models and make them user-friendly and then market them. This has received positive response in the Midwest region.

Comment: (Audience) You don't really need anything but the references. A user really needs to know PHYSICALLY what is going on, to get reliable results!

Comment: (G. Hart) I agree...to a point.

Comment: (K. Seip) The advent of better PC's will make it easier to write user-friendly models.

Comment: (Audience) An example is the Sediment-2 model, developed at Purdue University. It was developed by researchers and then Extension personnel took it and put it into a good form and put on seminars to train users.

Comment: (K. Baun, Wisconsin) What does User-Friendly mean? It is difficult to take a model to other locations. Write code that someone can modify for their situations. Data collection is the real problem. Write the model to read DBASE-II files, Lotus files, etc...THEN, it can be used by almost anyone.

Comment: (D. DeCoursey, USDA/ARS, Hydro-Ecosystems Research Unit, Fort Collins, Colorado) We need to work with users to make our product valuable. Users MUST BE INVOLVED UP-FRONT!

SUMMARY

The most vocal comments were regarding how to make current "research" models easier for the end user to implement. "Artificial Intelligence" and "Expert Systems" hold promise to assist in this pursuit. However, involving end-users in the early development of models is one of the best solutions. For those models that are already developed, end-users must be consulted before efforts to simplify the user-interface can be effective.

GROUNDWATER QUALITY MODELING FOR AGRICULTURAL NONPOINT SOURCES

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ABSTRACT

The various approaches for modeling agricultural nonpoint groundwater contamination are reviewed. A case history from The Netherlands is used to demonstrate and illustrate current modeling methodology. A method for considering risk and uncertainty in model analysis is outlined. It is shown that decision making regarding control of agricultural nonpoint contamination can be assisted by the use of current modeling methods.

INTRODUCTION

This paper is divided into four sections. The first section introduces basic modeling concepts. The second section reviews the state of the art of transport modeling in aquifers. The third section describes a case study in The Netherlands and the fourth section discusses risk assessment as it relates to modeling of nonpoint source pollution.

GROUNDWATER POLLUTION MODELING: AN INTRODUCTION

Mathematical modeling is used to describe quantitatively the mechanical, physico-chemical and biochemical phenomena characterizing pollution transport in the soil and the subsoil and to predict their evolution under various assumptions.

Pollution due to agricultural activities is probably the most difficult pollution to model because it is usually diffuse and governed by chemical and microbiological phenomena not well known or represented. Therefore only a few models have been developed specifically for application to agricultural pollution of groundwater. However, there exist numerous models of pollution transfer in porous media which could be used; Anderson (1979) presented surveys of these models. Our task is thus difficult as we face the alternatives - to produce a rather empty paper with the models actually in use or to write a book listing all applicable models.

Two more difficulties can be added - the variety of contaminants which must be considered, each with its specific chemical behavior, and the interrelationships between the soil and the subsoil which makes it unrealistic to treat the saturated and unsaturated zones separately.

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This paper attempts to provide some assistance in understanding which, among the parameters governing agricultural pollution, can be computed with present models and also what theoretical support, in addition to the already existing experimental support, mathematical modeling could offer for legislation and regulation of agricultural pollution.

The problem of nitrates is a most interesting example of agricultural pollution as it allows us to cover all aspects of modeling and, besides, is a subject for concern in most parts of the world. This is not to say that nitrates are the only or most important problem. Heavy metals, pesticides, and other chemicals used in modern agriculture are also of concern. However, we will focus our presentation on nitrates.

The categories of models can be classified with respect to the degree of knowledge we have of the underlying phenomena:

- (1) Budget models where only inputs and outputs are accounted for, without any assumption as to the structure of the phenomena,
- (2) Reservoir models, where some information on the structure of the phenomena is introduced,
- (3) Structural models, which use information on the structure of the phenomena which is as complete as possible, and which usually consist of transport and physico-chemical or/and biochemical models, usually coupled.

Budget Models

Budget (or black box) models simply relate outputs to inputs with or without an assumption of good mixing in the aquifers.

The simplest model computes the difference between the nitrogen input from the soil, the agricultural practice, or the atmosphere, and the nitrogen output by plant uptake, denitrification, and gaseous releases or exchanges with surface water. These outputs can usually be measured. This difference is interpreted as an estimate of the amount of nitrogen reaching the aquifer and contributing to pollution by nitrates. The various elements of the budget are related to a unit area and account for the different management techniques that are or may be practiced. A black-box model can be used at the local, regional or national scale and is represented by the following type of equation with units of [M] unless otherwise noted:

$$P_r + F_{ij} + K_1 H + Y + m X_1 = D_e + D_r + X_2 + E \quad [1]$$

where

P_r	=	rainfall,
F_{ij}	=	symbiotic and nonsymbiotic fixations,
K_1	=	the rate of humus decomposition [mass/time]
H	=	humus content,
Y	=	the fertilizer amount,
m	=	mineralization coefficient of organized nitrogen by the previous crop [dimensionless]
X_1	=	the amount of nitrogen contained in the previous crop,
D_e	=	denitrification,
D_r	=	drainage losses, and
X_2	=	the amount of nitrogen contained in the vegetal production,
E	=	gaseous losses.

This approach has been used in France. Other forms of this model exist which differ mainly in the way the budget terms are written and estimated. For instance, a model used in the United

Kingdom distributes the inputs between mobile and immobile forms of nitrogen and transforms them into outputs due to volatilization, plant uptake, denitrification and infiltration using an elementary empirical equation (in units of mass of nitrogen):

$$X_4 = \begin{cases} P (M - E_3 - X_3) & P \leq 1 \\ M - E_3 - X_3 & P > 1, \end{cases} \quad [2]$$

where $x_3 = f(D, M, P, n)$,
 $D = g(S, P, n)$,
 X_4 = the leached amount,
 P = the ratio of residual effective rainfall to the mean,
 M = the total mobile nitrogen,
 E_3 = the amount used by plants,
 X_3 = the denitrified amount,
 S = the total immobile nitrogen,
 n = the percentage of clay in the soil,
 f = an error function calibrated using experimental data found in the literature, and
 g = an exponential function based on experimental data on soil mineralization.

These models are quite elementary and do not require much mathematical knowledge. They enable one to estimate the amount of nitrate lost during a given period, generally a year; they also yield trends and regional differences. However, they are limited by the difficulties of estimating some of the terms in the budget, their lack of accuracy, their simplicity which precludes them from describing the mechanisms of leaching and therefore from predicting the results of modifications such as climatic changes and management practices. In a control strategy they allow a first choice of options and they are an aid in decision making.

Other models are not specific to agricultural pollution but could probably be used successfully. Some are based on probabilistic transfer functions calibrated by field tests to determine travel times to a given depth (Jury 1982). Others involve a statistical analysis of input-output (cluster or canonical analysis) to identify preferential hydraulic paths in a given area or the introduction of signal theory methods like deconvolution.

Reservoir Models

Reservoir models are derived from budget models and allow some quantification without introducing a structural description of the transport phenomena in the saturated and unsaturated zones.

The basic idea is to divide the path traveled by a contaminant into cells or reservoirs where the contaminant mixes with and is diluted by groundwater; the contaminated water migrates from one reservoir to another and is continuously diluted. Some models consist of a single reservoir only and others are based on a sequence of reservoirs.

For example, a model developed in the United Kingdom to represent the movement of nitrates in the English chalk, is a bidimensional reservoir model where nitrates reaching the water table are assumed to completely mix with nitrates already present in the saturated zone. In this approach, the time step is one year and a typical cell is 500 m square. The input data are the annual recharge, the history of soil use, fertilizer application rates, the distribution of groundwater levels and pumping rates, the depth to the water table, water contents in the unsaturated zone, and the effective depth of flow in the saturated zone. For a year of simulation, the following computations are performed:

- (1) ground water flow rates are estimated from the distributions of water levels, recharge and pumping rates;
- (2) at each node, the nitrate flux to the water table is estimated either as the output from a vertical movement model or it is based on soil use data. Then a time delay is introduced which is a function of the water content and the thickness of the unsaturated zone and the recharge rate.
- (3) nitrate concentrations in the aquifer are then estimated under the assumption that the nitrates coming from the unsaturated zone or transported by ground water completely mix with nitrates already present in the saturated zone over its entire depth.

This model has been used to simulate nitrate concentrations in pumping wells.

Reservoir models account for only one physical phenomenon, advection, during transport in the saturated and unsaturated zone; dispersion is neglected. All other aspects are ignored, more particularly the porous-medium structure which governs the mixing process. For the long range, and for aquifer volumes large enough, it can be assumed that the measured concentration is not much different from that computed using the assumption of instantaneous mixing. For short term or local situations the approximation is much greater. Therefore, we feel that reservoir models should not be used in a short term control strategy. However, at a site where it has been calibrated, and for long enough times and slowly varying inputs, a reservoir model is a forecasting tool which is more accurate than budget models and therefore a better decision aid.

Structural Models

Structural models are complete models which try to account for all elementary processes (e.g. mechanical, physico-chemical and biochemical, and biological), usually by means of partial differential equations. They are generally very complex and their solution most often be numerical. They may be difficult to use because they require many parameters which may be hard to measure.

Structural models can be classified into three categories: physico- and biochemical models, biological models, and transport models. The first two categories are used to estimate the quantity of nitrates available for leaching and are coupled to transport models providing boundary conditions in the form of input concentration values or source terms. These models are presented in other conference papers; however, to provide a complete view of non-point modeling, we will briefly outline their main features.

Physico-chemical and Biochemical Models

Their purpose is to provide a quantitative estimate of the nitrates produced from the reactions governing the transformations of nitrogenous compounds in the soil and subsoil in order to compute the amounts of nitrates which could possibly be leached and transported in the soil and subsoil.

ANIMO (Rijtema et al. 1988), which is used in The Netherlands case study presented later, is a structural model which simulates the behavior of nitrogen and organic carbon in a soil-water-plant system, considering:

- (1) soil type
- (2) soil use
- (3) water management
- (4) weather conditions
- (5) fertilizer use
- (6) cropping history

The model uses a one dimensional soil system divided into a number of horizontal layers. In its present form it can be used either at a field or regional scale. If we consider the top soil as the part of the soil zone where agricultural activities are concentrated, the nitrogen balance for this system can be represented as shown in figure 1.

Inputs of nitrogen can originate from fertilization, both organic and inorganic, and soluble N forms in precipitation. In the soil-water-plant system the different forms can be transformed one to another, and some can be transported to deeper layers. These processes are influenced by environmental factors such as temperature, moisture, aeration and pH. The processes and their influencing factors are quantitatively described in the model. Nitrogen can leave the topsoil due to harvesting, leaching to deeper layers, and by volatilization. Nitrogen can be present in different forms in the soil, and the various forms can be transformed through the processes in the nitrogen cycle as shown schematically in figure 2.

To quantify these processes it is necessary to quantify the processes in the carbon cycle because of the many interdependences between organic material and nitrogen. The simplified soil organic matter or carbon cycle used in the model is shown in figure 3.

In ANIMO, attention is focused on the following processes:

- (1) mineralization/immobilization of N in relation to formation and decomposition of different types of organic matter as organic fertilizer, root material, root exudates and native soil organic matter;
- (2) denitrification in relation to (partial) anaerobiosis and the presence of organic matter;
- (3) transport, formation and decomposition of NO_3 , NH_4 , and soluble organic matter.

ANIMO has been extensively tested using measured data from long-term fertilization experiments on grassland and forage corn. These tests considered:

- (1) nitrogen uptake by the crop
- (2) mineral nitrogen in the soil solution
- (3) total nitrogen in the soil
- (4) leaching from the rootzone to groundwater

An example of model validation is shown in figure 4 where model calculations have been compared with measured data under a forage corn field fertilized for 9 years with 250 tons of cattle slurry per ha per yr.

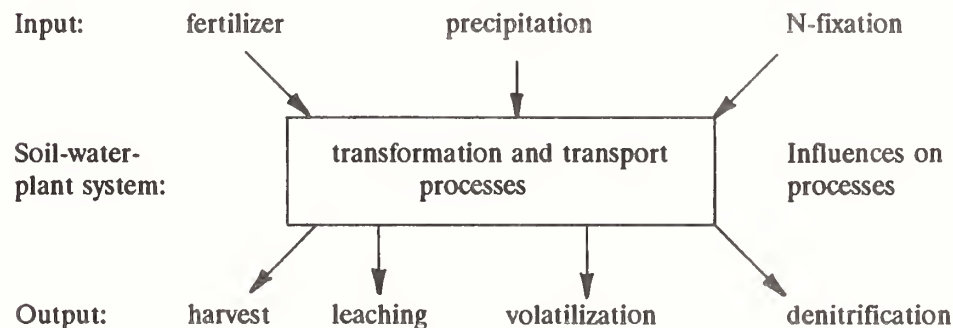


Figure 1.
Nitrogen balance for the topsoil.

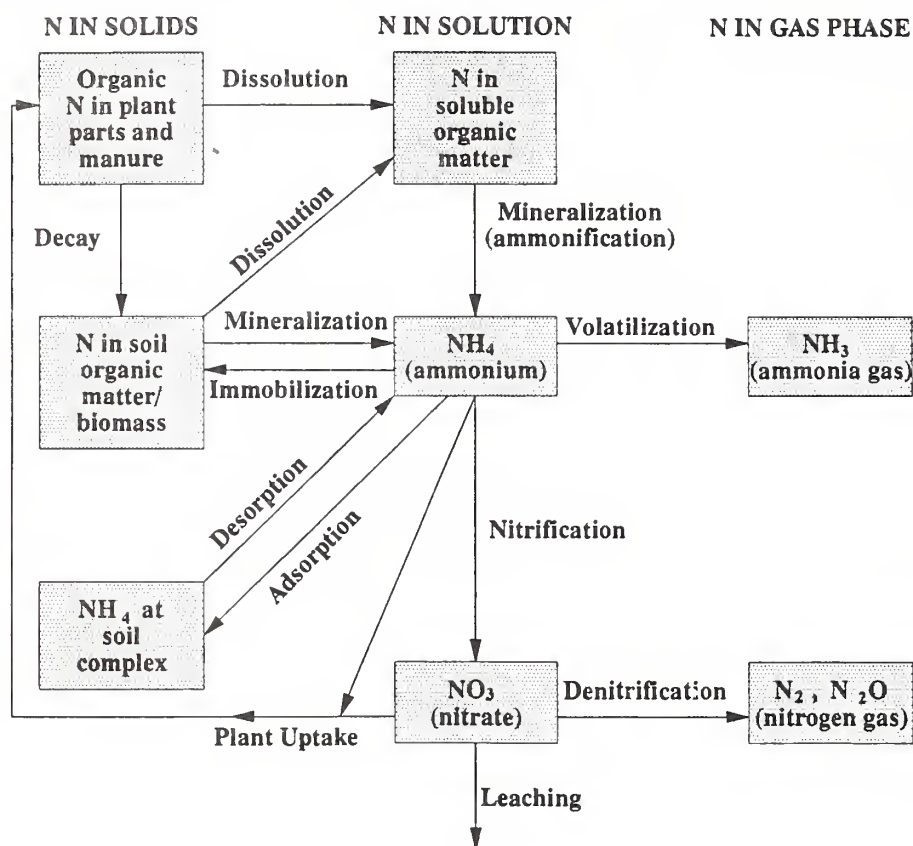


Figure 2.
The nitrogen cycle.

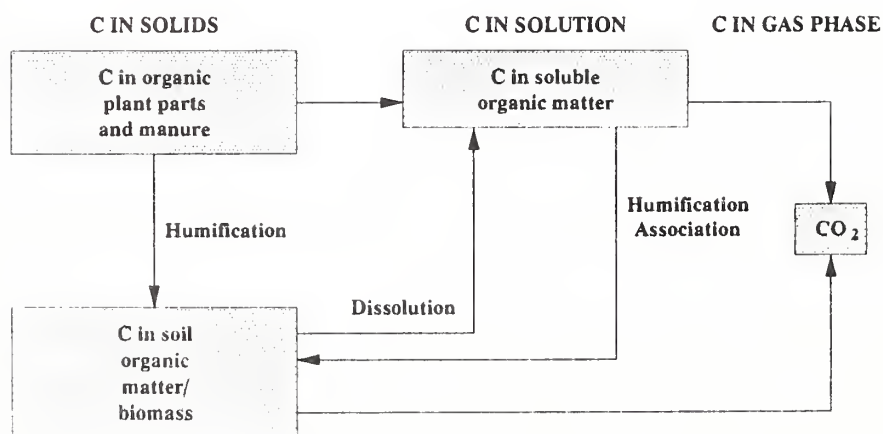


Figure 3.
The carbon cycle.

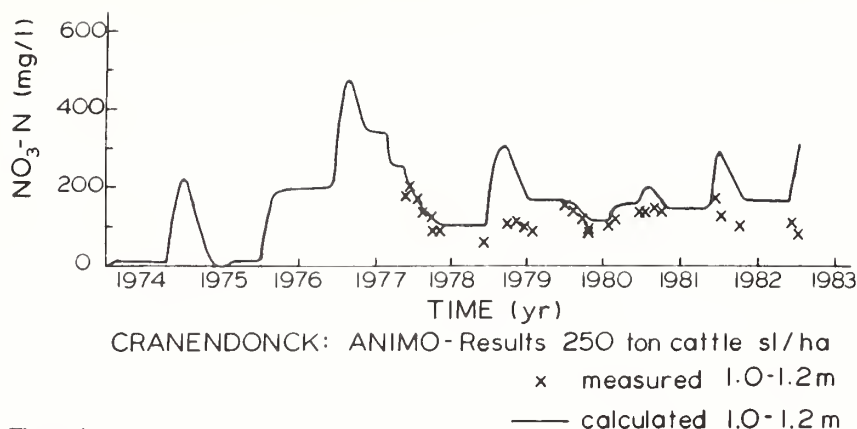


Figure 4.
Calculated and measured $\text{NO}_3\text{-N}$ concentration at a depth of 1.0 - 1.2 m
below soil surface under a forage corn field, with cattle slurry
application of $250 \text{ t/ha}^{-1}/\text{yr}$.

Transport Models

Transport models have been developed in rather great numbers since the late sixties for groundwater pollution studies but very seldom to treat the case of nonpoint sources. They usually consist of a hydrodynamic module (water flow as a pollution vector), a hydrogeologic module (relationships between biology, lithology, rainfall and flow), and a physico-chemical module (molecular diffusion, sorption, and chemical reactions).

Transport takes place with some spreading of the contaminant and at velocities different from those of pure water; this is dispersion, which can be accounted for or neglected, depending on the scale at which the phenomena are considered. It is usual to distinguish between transport in the unsaturated-zone, mainly vertical, and transport in the saturated zone, mainly horizontal. They are coupled by introducing the outputs of unsaturated zone models as inputs, boundary conditions or source terms for saturated zone models.

Transport is modeled by the general advective-dispersive equation, which, in the saturated zone, can be written as:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial c}{\partial x_j} \right) - V_i \frac{\partial c}{\partial x_i} + G \quad [3]$$

where x_i = spatial coordinates,
 t = time,
 C = concentration,
 V_i = pore velocity,
 D_{ij} = dispersion tensor,
 G = source or sink term representing exchanges of contaminant with the unsaturated zone or other aquifers.

In the following sections, we review some of the characteristics and forms of this equation, starting with a simplification for purely advective transport when dispersion is neglected, and ending with more sophisticated models based on a stochastic approach.

SATURATED-ZONE CONTAMINANT TRANSPORT MODELS

Once a nonpoint source contaminant reaches the saturated soil zone it can migrate for large distances, thereby becoming a potential threat to water resources or environmentally sensitive

areas. In the course of its migration through the groundwater system, the contaminant is subjected to processes such as hydrodynamic dispersion and geochemical transformations involving constituents present in the soil. These processes will affect the nature and severity of the contamination to be expected at points downstream of the source. Because migration paths may lead through various hydrogeologically and geochemically different soil zones, the resulting contamination may depend upon the path taken by the contaminant.

An example illustrating the importance of the local geochemistry is the Fuhrberger Feld aquifer near Hannover in Germany (Koelle et al. 1985, Strebel et al. 1985). The aquifer is exposed to high nitrate input from agricultural activities. Upon entering the saturated zone, the nitrate is reduced by reaction with pyrite which is present in the soil, producing nitrogen gas and sulphate. Below a certain depth the sulphate is further transformed by reaction with organic carbon. As a consequence, water withdrawn by wells situated downstream of the input zone contains more sulphate than nitrate. The amount of the various contaminants found in the well water depends on the migration paths and the availability of reactants along these paths.

A structural model must therefore be capable of giving a valid representation of, first, the flow system, and second, the physical and geochemical processes acting on the contaminant during its migration along the flow paths. Models of this type are often used in sensitivity analyses, where parameters that are uncertain are varied within a certain range and the model response is observed. Provided it is based on a physically valid representation of the relevant processes, a model used in this way can provide valuable insight into the likely fate of contaminants even in situations where hydrogeologic data are lacking.

The groundwater flow system and contaminant migration paths can be defined either in three dimensions, or in two dimensions in the vertical cross-sectional plane. Fortunately the diffused nature of the source reduces the importance of transverse dispersion, and renders a fully three-dimensional representation less important than in the case of point sources. A vertical cross-sectional model oriented along the water table gradient is therefore a good choice for the study of transport of nonpoint-source contaminants.

The relevant processes for contaminant transport in the saturated zone are advection by the moving groundwater, dispersion due to the soil microstructure and heterogeneities, molecular diffusion, adsorption, and geochemical reactions. Because concentrations of non-point source contaminants are generally low, density effects can be neglected.

Groundwater Flow and Advective Transport

Several methods are available for the simulation of advective transport. Most methods involve the solution of the groundwater flow equation (Bear 1979) for hydraulic head and the subsequent application of Darcy's equation to calculate flow velocities. The velocities are then used in a numerical model such as the method of characteristics or the particle tracking method (see Kinzelbach 1986) to simulate advection. This approach is appropriate when hydraulic gradients are reasonably large, which is normally the case in systems containing pumping or recharge wells. If gradients are small however, as in the case of a natural flow system in a low-relief crop land area, the approach may not be sufficiently accurate with respect to the delineation of migration paths.

A method that is better suited for such situations is the dual approach involving both hydraulic potential and stream functions (Frind and Matanga 1985, Frind et al. 1985) to formulate the flow problem. The method produces highly accurate flownets directly and thereby provides immediate insight into the nature of the flow system and the contaminant migration paths. Although the theory assumes steady-state flow, seasonal transients can be accommodated through a series of instantaneous steady states.

For steady flow in two dimensions, assuming that the coordinate axes (x,y) are aligned with the principal directions of hydraulic conductivity, the dual governing equations for the hydraulic potential $\phi = \phi(x,y)$ and the stream functions are

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial \phi}{\partial y} \right) = 0 \quad [4]$$

$$\frac{\partial}{\partial x} \left(\frac{1}{K_{yy}} \frac{\partial \psi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{1}{K_{xx}} \frac{\partial \psi}{\partial y} \right) = 0 \quad [5]$$

where K_{xx} and K_{yy} are the principal components of the hydraulic conductivity tensor. The boundary conditions (figure 5) on these two equations are given either in terms of a specified value of the respective variable itself (first type) or of its derivative (second type). The first-type boundary conditions are of the form:

$$\phi = \phi_0(\Gamma) \text{ on } \Gamma_1 \quad [6]$$

$$\psi = \psi_0(\Gamma) \text{ on } \Gamma_2 \quad [7a]$$

where Γ_1 and Γ_2 are parts of the boundary Γ . Equation 7a can also be expressed in terms of a boundary flux q_0 in the form:

$$\psi(\Gamma) = \psi_0(\Gamma_0) + \int_{\Gamma_0}^{\Gamma} \bar{q}_0 \bar{n} d\Gamma \quad [7b]$$

where \bar{n} is the normal vector at the boundary. The second-type boundary conditions, expressed in terms of the boundary gradients \bar{g}^ϕ and \bar{g}^ψ , are of the form:

$$\bar{g}^\phi \bar{n} = \bar{q}_0 \bar{n} \quad [8]$$

$$\bar{g}^\psi \bar{n} = -\nabla \phi \bar{r} \quad [9]$$

where \bar{r} is the tangential vector at the boundary. The numerical solution of equations 4 and 5, together with the appropriate boundary conditions, produces a flownet as shown in figure 6.

Once the flownet is defined, estimates of advective transport can be made simply by tracking along the streamlines. The travel time, $t(s)$, taken by a particle to travel the distance between two points s_0 and s on a streamline is given by

$$t(s) = \frac{\theta}{\Delta\psi} \int_{s_0}^s \Delta p(s) ds \quad [10]$$

where θ = the effective porosity,
 $\Delta\psi$ = the stream function interval, and
 $\Delta p(s)$ = the streamtube width.

The travel time is thus simply the area of the streamtube between the starting point and the target point, multiplied by a constant.

Because the stream function interval, $\Delta\psi$, represents the discharge in a streamtube, discharge fluxes at outflow boundaries, such as stream or lake bottoms, are obtained directly from the stream function solution.

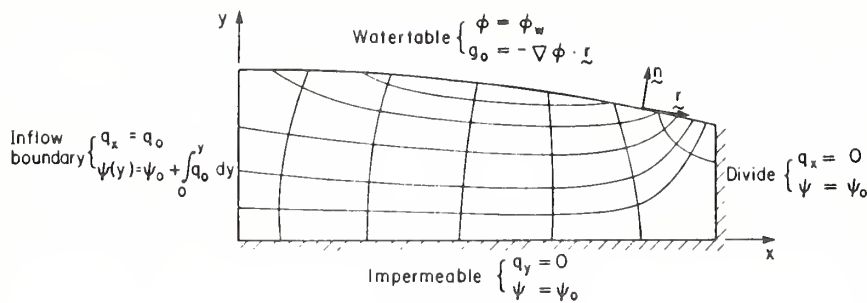


Figure 5.
Dual boundary conditions for
steady-state flow system.

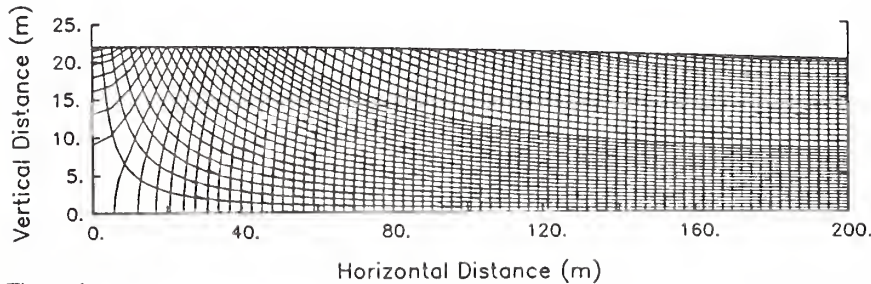


Figure 6.
Typical flownet from potential-stream function model.

Flow models, both those of the dual type and the conventional potential-based type, are now at a mature stage of development and are used extensively in aquifer contamination studies.

Advective-Dispersive-Reactive Transport

For sand and gravel aquifers, the most relevant processes affecting contaminant transport, in addition to advection, are hydrodynamic dispersion and geochemical transformations. Dispersion is relevant particularly in natural systems with long migration pathways because the resulting spreading will cause first arrivals of contaminants in sensitive locations earlier than indicated on the basis of advection alone.

Reactions taking place between the contaminant and geochemical constituents present in the soil can be highly complex, involving multiple components taking part in equilibrium as well as kinetic reactions. For simplicity, we will consider here only an exponential decay type reaction, as well as linear adsorption. The decay reaction may represent, for example, denitrification by reaction of nitrate with sulphur to produce sulphate and nitrogen gas.

Assuming isothermal conditions, a non-deforming medium, the absence of significant density differences, as well as the absence of sources and sinks, the governing differential equation takes the form:

$$\frac{\partial}{\partial x_i} \left(\frac{D_{ij}}{R} \frac{\partial c}{\partial x_j} \right) - \frac{v_i}{R} \frac{\partial c}{\partial x_i} - \lambda c = \frac{\partial c}{\partial t} \quad [11]$$

where x_i = spatial coordinates,
 D_{ij} = hydrodynamic dispersion tensor, and
 t = time,
 c = $c(x_i, t)$ = concentration of the contaminant,
 v_i = average linear pore water velocity,
 λ = $(\ln 2)/t_{1/2}$ = the decay constant, with $t_{1/2}$ being the half-life

standard textbooks (see for example Pinder and Gray 1977 or Kinzelbach 1986). Since numerical solutions of the advection-dispersion equation are subject to numerical dispersion, it is important that the spatial and temporal discretization be designed such that the well-known Peclet and Courant criteria are satisfied. A detailed procedure for the design of grids is given by Frind and Germain (1986).

Figure 7 shows the evolution of a typical plume of a non-reactive contaminant in a sandy aquifer. The contaminant originates at a narrow nonpoint source. Equations 4, 5, and 11 were used in the solution.

Although conventional dispersion theory considers the dispersion coefficient to be a characteristic parameter of a given porous medium, it is now generally recognized that this parameter depends on the scale of the system. Recent advances in the stochastic theory of dispersion for heterogeneous media (see for example Gelhar and Axness 1983) have contributed greatly to the understanding of scale-dependent dispersion. Stochastically-based techniques that relate the dispersive parameters directly to measurable statistical properties of the aquifer material have also been developed (Sudicky 1986). In the light of these theories, the dispersion coefficient defined in equation 13 may be interpreted as relating to the asymptotic value that is reached after the plume has traveled a sufficient distance in a heterogeneous but statistically homogeneous porous medium.

For more complex kinetic and equilibrium reactions involving multiple constituents, general geochemical models (see for example Parkhurst et al. 1980) have been developed. Models of this type generally focus on the local geochemical processes without consideration of advection and dispersion. A major obstacle to the linking of general geochemical models and dynamic transport models up to now has been the large demands on computing power; this obstacle is now being overcome and some promising work has appeared in the literature. Narasimhan et al. (1986), for example, have combined the geochemical model PHREEQE with a numerical transport model to

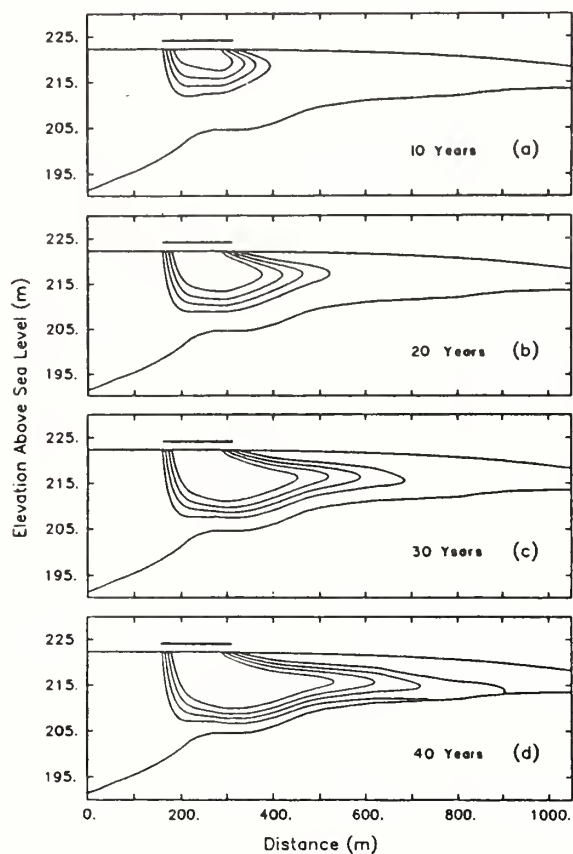


Figure 7. Evolution of the Borden plume to 40 years; third type boundary condition, constant source concentration; contour interval 0.2 relative concentration (after Frind and Hokkanen 1987).

The linear adsorption process is represented by the retardation coefficient R (Freeze and Cherry 1979), defined as:

$$R = 1 + \frac{\rho_b}{\theta} K_d \quad [12]$$

where ρ_b = the bulk density of the saturated porous medium,
 K_d = the distribution coefficient that governs the partitioning of the solute into dissolved and adsorbed phases, and
 θ = the effective porosity.

The hydrodynamic dispersion tensor D_{ij} is defined, according to Bear (1979), as:

$$D_{ii} = \alpha_L \frac{v_i^2}{\bar{v}} + \alpha_T \frac{v_j^2}{\bar{v}} + D^* \quad [13a]$$

$$D_{ij} = D_{ji} = (\alpha_L - \alpha_T) \frac{v_i v_j}{\bar{v}} \quad [13b]$$

where v_i = the velocity components in the respective directions,
 $\frac{\bar{v}}{\bar{v}} = (\sum v_i^2)^{1/2}$
 α_L = the longitudinal dispersivity,
 α_T = the transverse dispersivity, and
 D^* = the effective molecular diffusion coefficient.

The boundary conditions in equation 12 can be either of the following: The first (Dirichlet) type is

$$c = c_0 \text{ on } \Gamma_1 \quad [14]$$

where c_0 is a specified concentration. The second (Neumann) type is

$$\frac{\partial c}{\partial \bar{n}} = \bar{g}_n \text{ on } \Gamma_2 \quad [15]$$

where \bar{n} is the unit vector normal to the boundary (inwards positive) and \bar{g}_n is a specified concentration gradient. The third (Cauchy) type is

$$v \bar{n} c - D_{\bar{n}} \frac{\partial c}{\partial \bar{n}} = \frac{\bar{q}_n c_0}{\theta} \text{ on } \Gamma_3 \quad [16]$$

where the left-hand side contains the advective and dispersive mass fluxes normal to the boundary and \bar{q}_n is a known Darcy flux normal to the boundary. The term $\bar{q}_n c_0 / \theta$ is positive if it adds mass to the system. The boundary of the solution domain is $\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_3$. The Neumann boundary condition with a gradient of zero is normally used at impermeable boundaries. The solution also requires the provision of suitable initial conditions.

The governing differential equations can be solved by various numerical methods such as finite differences or finite elements. In these methods, the physical domain is discretized into elements or cells, and the solution is found at a number of nodal points. The procedures are described in

handle the simultaneous migration of several reacting constituents. Most recently, Herzer (1988) developed a finite-difference based dual-porosity transport model capable of handling ion adsorption and denitrification processes with either fast or slow reactions.

Advective-dispersive models for two dimensions are now at a fairly mature stage of development, and numerous proven codes are in existence. Most of these models can be run on advanced microcomputers. For three dimensions, development is much less advanced, and applications to real systems have so far been limited.

Advective-Diffusive Transport

For aquifers containing zones of stagnant water, as for example in the case of a sandy aquifer containing clay lenses, the interaction between advective and diffusive processes plays an important role (Gillham et al, 1984). Models that recognize this interaction are known as dual-porosity models. The diffusive transfer into or out of stagnant zones will retard the front of a contaminant plume and cause a tailing effect that cannot be obtained with an advection-dispersion model alone, except at the microscale (Frind et al. 1987).

The governing differential equation for advective-diffusive transport is formulated in a form analogous to that for advective-dispersive transport. Approximating the diffusive exchange as a first order process (van Genuchten and Wierenga 1976), the governing differential equations, excluding reactions, become:

$$\theta_m \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial c_m}{\partial x_j} \right) - \theta_m v_i \frac{\partial c_m}{\partial x_i} = \theta_m \frac{\partial c_m}{\partial t} + \theta_s \frac{\partial c_s}{\partial t} \quad [17]$$

$$\alpha(c_m - c_s) = \theta_s \frac{\partial c_s}{\partial t} \quad [18]$$

where c_m and c_s = the concentrations in the mobile and stagnant regions, respectively,
 θ_m and θ_s = the volumetric water content of the mobile and stagnant regions, respectively,
 v_i = the average linear velocity in the mobile region, and
 α = a first-order mass transfer coefficient.

The boundary conditions are the same as those for the advection-dispersion model.

The dual porosity transport model holds considerable promise because of its more physically realistic representation of the transport mechanism. Analytical as well as numerical solutions have been developed, but applications so far have mainly been confined to the research sphere. More work needs to be done to demonstrate the utility of this type of model in practical situations.

A CASE STUDY IN THE NETHERLANDS

In The Netherlands the demand for good quality water for agriculture, industry, municipal water supply and for nature reserves is steadily increasing. For municipal and industrial water supply the main objective is to have a sufficient supply of good quality surface and groundwater.

In many regions, agriculture is the dominant activity both in its economic value and in its impact on groundwater quality. Intensification in agriculture has led to an increased fertilizer use. The potential for livestock waste to pollute surface waters and groundwater is high, particularly when

animal slurries are applied in excess of crop requirements. The extent of the slurry disposal problem was not recognized in the early stages of intensive farming. In particular, difficult soil and drainage conditions on parts of a farm may limit the area suitable for landspreading in winter, leading to local over-applications.

This condition exists in the western and southern part of The Netherlands, where land elevation ranges between 5 and 30 m above sea level. Surface drainage is provided by an irregular network of natural brooks, and ditches and open field drains created for agricultural purposes, of which only the major ones discharge throughout the year. Beneath the surface, Pleistocene sands form a thick and highly permeable aquifer.

The average precipitation in the area is about 750 mm fairly regularly distributed over the year. The annual evaporation is about 450 mm. During the summer, precipitation is, on the average, balanced by evapotranspiration so that the precipitation excess of about 300 mm occurs during the winter period. About 80 percent of this precipitation excess discharges during the winter and about 20 percent as summer baseflow discharge.

The groundwater table is high, averaging about 40 cm below the ground surface in winter and about 130 cm in the summer. Insufficient capacity of the drainage system, although locally narrowly spaced, can cause inundation and surface runoff in the lower parts of the area after excessive precipitation.

Deep well pumping of groundwater from thick phreatic aquifers or semiconfined aquifers causes declines in the phreatic level. Primarily this results in less baseflow.

Description of Pilot Region

The pilot region of 35,000 ha is located in the southern part of the Netherlands in the province Noord-Brabant. The "Peelrand" fault divides the area into two hydrologically different regions. West of the fault (de Slenk) there are three main aquifers of coarse sand separated by layers of clay, peat and clayloam. The hydrologic basement is about 300 m below land surface. East of the fault (de Horst), the basement is only 8-35 m below land surface. The aquifers are overlain in both regions by fine sands with a thickness of 25 m in the Slenk and 5 to 10 m in the Horst. The surface layers have an average organic matter content of .4%; the first aquifer in the Slenk has .08%, and the Horst .06%.

Deep-well pumping for municipal water supply occurs at two locations, with an abstraction of 4,500,000 m³/yr at the first and 3,000,000 m³/yr at the second, respectively. Additional deep well pumping for municipal water supply is planned. Groundwater abstraction for industrial purposes amounts to 1,500,000 m³/yr.

Agriculture can be characterized by an intensive use of fertilizers, with a need for both good drainage in winter and an additional water supply in summer. Agriculture in the region is very intensive, with a stocking rate of 4 standard livestock unit dairy cows per ha grassland, and a density of 20 pigs and 230 chickens per ha of agricultural land.

Model System

The model ANIMO discussed in the first section is applied here on a regional scale, using output from the external water management model SIMGRO as input. Coupling with other water quantity models is possible, provided that these models also consider the unsaturated zone.

The model SIMGRO (Querner and Van Bakel 1984, Querner 1988), has been developed to simulate flow in the saturated and unsaturated zones. The effects of irrigation including its impact

on the surface water system is also included. The saturated zone module consists of a quasi-three dimensional finite element model using an implicit calculation scheme. The unsaturated zone is modelled as two reservoirs, one for the root zone and one for the subsoil. Storage of water in the root zone is considered along with extractions and inflows. From the subsoil water balance, the phreatic surface elevation is calculated using the storage coefficient.

The unsaturated zone is related to land-use technology on a subregional level. Subregions are chosen to have relative uniform soil properties and hydrologic conditions.

The various water movements considered within a subregion are shown in figure 8.

Practices and Policies

The following practices were considered in the model calculations to evaluate their agricultural effects:

- (1) intensively used grassland, with day and night grazing, with and without supplemental sprinkling irrigation;
- (2) arable land with a crop rotation of cereals, potatoes, sugar beet with and without supplemental sprinkling irrigation;
- (3) forests;
- (4) nature reserves;
- (5) urban areas.

In conjunction with a general soil protection law, the government has introduced regulations for the use of animal slurries in agriculture. In addition to a prohibition of landspreading of animal slurries from November 1st to March 1st, applications of animal slurries are restricted to a maximum phosphate amount to prevent dumping of animal slurries on agricultural lands. The maximum phosphate level is to be reached in four timesteps of four years. The restrictions are given in table 1.

In the P_0 phase it is assumed that all animal slurries produced in the region are spread on agricultural land in the region, resulting in considerable loading on forage corn land.

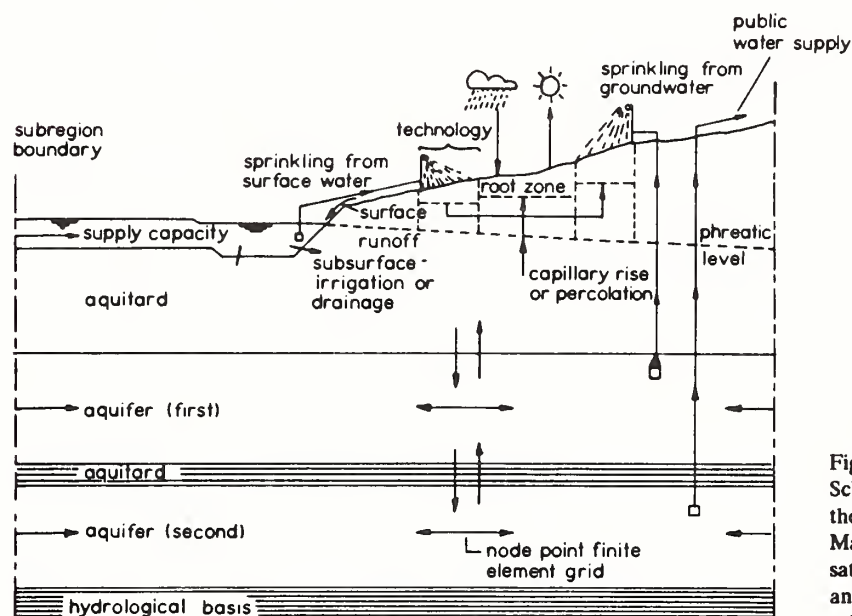


Figure 8.
Scheme of water management in the groundwater model SIMGRO. Main feature is the integration of saturated zone, unsaturated zone and surface-water system within a subregion.

Table 1.

Allowable levels of phosphate applications in kg P_2O_5 /ha/yr according to the regulation for application of animal slurries. P_0 indicates the present situation without restrictions.

Phase	Commencing Year	Application Rate		
		Arable Land	Forage Corn	Grassland
P_0	before 1987	free	free	free
P	1987	125	350	250
P	1991	125	250	200
P	1995	125	175	175
P	2000	70	75	110

In the analysis, special attention will be given to the effects of intensive agriculture and restrictive measures in agriculture, as well as the effect of deep wellpumping, on nitrate levels in the aquifer. To those ends an analysis of the following policies has been made:

- Scenario A: Continuation of the present level of landspreading of animal slurries till the year 2013 respectively 2043 with groundwater abstraction at the 1982 level.
- Scenario B: Landspreading of animal slurries starting at the 1982 level and reduced in phases according to Table 1 with additional application of inorganic nitrogen fertilizer as necessary; the groundwater abstraction remains at the 1982 level.
- Scenario C: Landspreading and fertilization as in scenario B but an increase in the present groundwater abstraction.

Determination of Initial Conditions

On the basis of an assumed initial nitrogen distribution in the soil profile in 1953 the present condition has been calculated using data on land use development and intensity of fertilization after 1953 as input. The calculated nitrate concentrations at different depths for the present (1983) situation are given in figure 9. The measured data at different depths under various land uses are given in table 2, showing a similar distribution with depth.

Some Results

Scenarios A and B were calculated for a period of 60 years to see if a steady-state situation between fertilization and nitrate leaching would be reached in the deeper layers. Scenario C was simulated for a period of 30 years, to see the effect of additional deep-well pumping on nitrate levels.

Table 2.

Measured concentrations of $\text{NO}_3\text{-N}$ in $\text{g}\cdot\text{m}^{-3}$ at various depths given as regional average and the average values under corn, grassland and nature. Number of observations = (40).

Depth (m)	Average $\text{NO}_3\text{-N}$ Concentrations in $\text{g}\cdot\text{m}^{-3}$			
	Regional	Corn	Grass	Nature
1- 5	13 (131)	54 (13)	21 (41)	1 (70)
5-10	1 (40)	2 (4)	2 (26)	0 (7)
10-15	2 (36)	4 (7)	2 (21)	0 (3)
15-20	1 (34)	2 (5)	3 (8)	0 (9)
20	.5 (46)	0 (8)	2 (13)	0 (20)

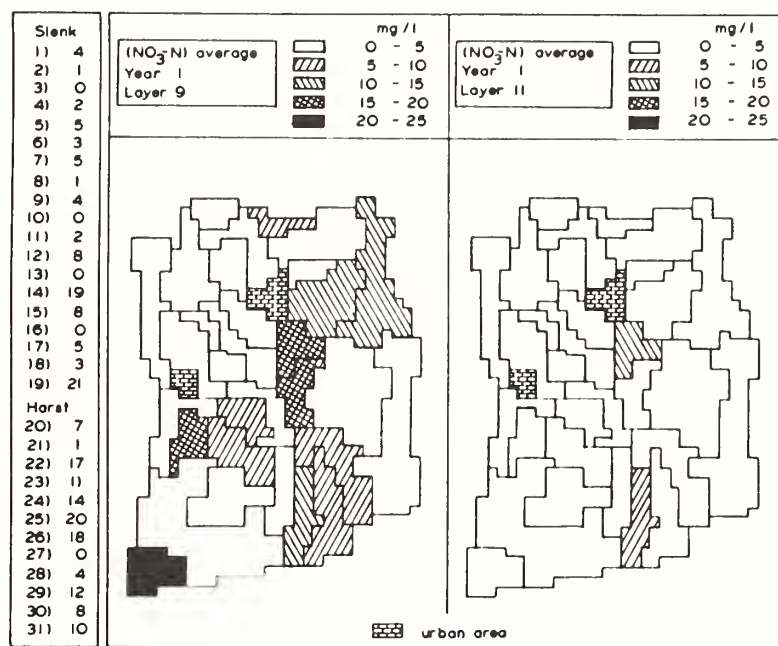


Figure 9.

Nitrate contents ($\text{mg NO}_3/\text{l}$) in the layers 9 and 11 as subregional mean values after simulation of historical development (= initial condition of February 1983 for policy analysis)

left layer 9

Slenk 1.5 - 6.0 m depth

Horst 1.5 - 6.0 m depth

right layer 11

Slenk 15.0 - 25.0 m depth

Horst 3.5 - 12.3 m depth

Figure 10 shows, for subregion 25, the relation between nitrate concentration and time for scenarios A and B at a depth of 3.5-5.1 m below the surface. From this result, it appears that the effect of a reduction of landspreeding at this depth lags the change by about 6 years.

In figure 11, the effect of a reduction in landspreading is compared with the non-restricted situation for the layer 1.5-6.0 m below the surface after 30 years. The scenario B nitrate concentrations in all subregions are considerably lower than for scenario A.

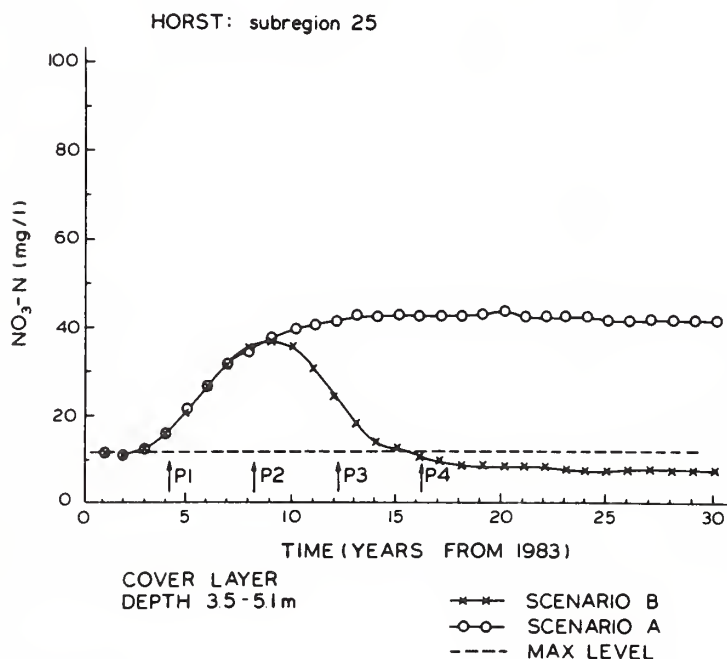


Figure 10.
Time dependency of NO₃-N at 3.5-5.1m depth as mean value in subregion 25 for the scenario's A and B. Arrows indicate the time of introduction of the various restrictions in slurry application.

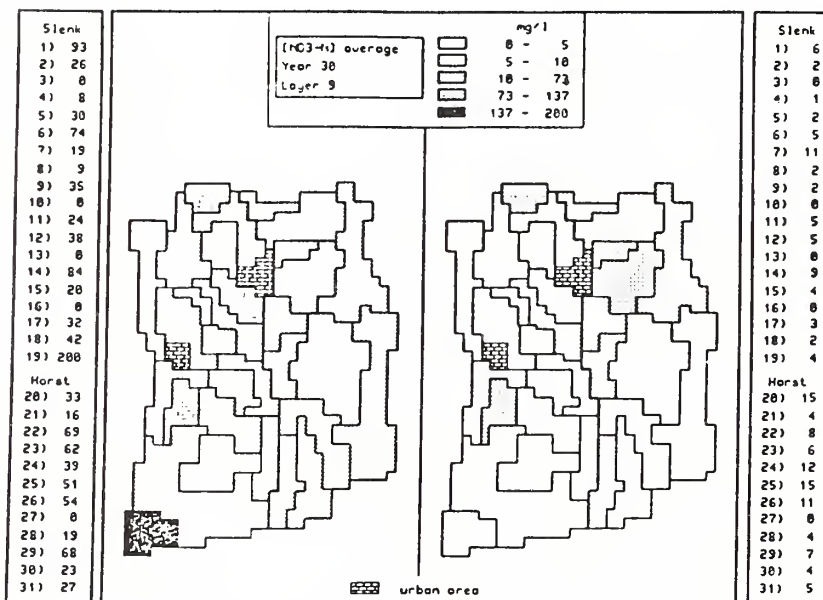


Figure 11.
Mean NO₃ concentration per subregion at 1.5-6.0 m depth after 30 years of simulation. Left Senario A, right Scenario B.

Simulations at longer times indicate that in most of the subregions after 30 years a reasonable steady-state situation has been reached. The stability of organic matter in the surface layer and in the aquifer plays an important role in denitrification. The significant reduction in nitrate concentration with depth is due to the relatively high organic matter concentrations in the deeper layers.

On the basis of the C/N ratio a decomposition rate of 0.00141/yr has been derived, reducing the quantity of organic matter by 50 percent in 500 years. Calculations of concentration in the deeper layers appears to be strongly dependent on the decomposition rate as is shown in figure 12 for a depth of 1.5 to 6.0 m below surface.

Calculations have also been made for other half-lives to show the effect of the stability of the organic matter in deeper layers on nitrate leaching.

In scenario C, additional deep well pumping for municipal water supply was introduced in Slenk subregion 12 with an abstraction of 5,000,000 m³/yr from the upper aquifer and 3,000,000 m³/yr from the lower aquifer. An additional 3,000,000 m³/yr of deep well pumping is introduced in subregion 25 in the Horst. The upper aquifer in subregion 12 is at a depth of 25.0-75.0 m below the surface, whereas the aquifer depth in subregion 25 is at 5.1-25.1 m depth.

The effects of the additional deep well pumping is concentrated in subregions 12 and 25 with an increase in the water table of 50-70 cm, whereas in the neighboring subregions hardly any effect could be demonstrated. The effect of additional deep well pumping on the nitrate concentration at a depth of 1.5-6.0 m below the surface is in the order of 20-25 percent increase, compared with scenarios B and C.

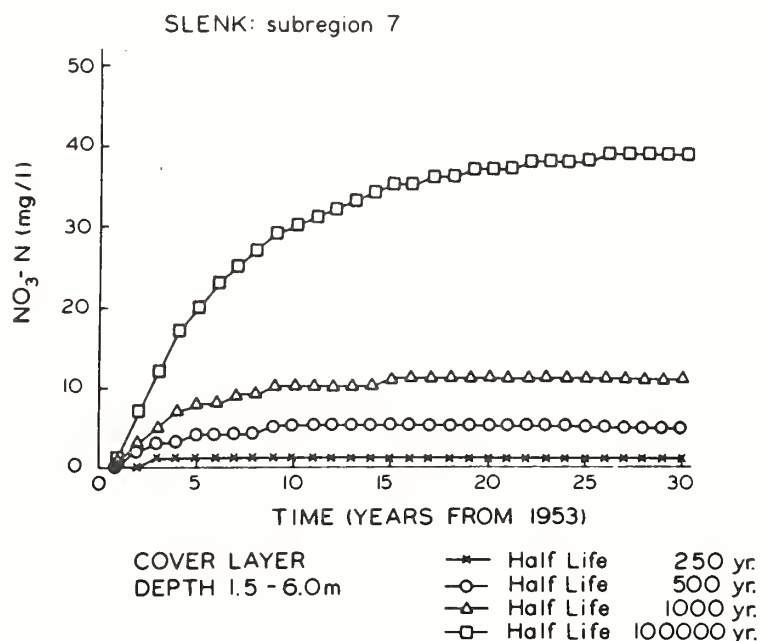


Figure 12.
Effect of stability of organic matter at 1.5-6.0 m depth, indicated by half-life on the development of the NO₃-N concentration in subregion 7 with time.

A FRAMEWORK FOR RISK ASSESSMENT OF NON-POINT POLLUTION

Problem Formulation

A risk analysis for nitrate contamination of groundwater can be formulated with:

- (1) the exposure being the level of nitrate in the ground water,
- (2) the probability density function of the exposure, and
- (3) the consequence of an exposure which may be analyzed with hazard identification and dose-response assessment methodologies (National Research Council, 1983).

Hazard identification is the process of determining if the exposure to an agent can cause an increase in the incidence of a specific health condition (cancer, birth defect, etc.). Dose-response assessment is the process of characterizing the relation between the dose, in this case the level of nitrate contamination, and the incidence of the adverse health effect in the exposed population.

The distinction between risk assessment and risk management follows the National Research Council (1983) definition. Risk assessment means the characterization of adverse effects caused by the exposure for a given (existing) situation. Risk assessment also includes characterization of the uncertainties inherent in the process of inferring risk. Risk management describes the process of evaluating alternative control strategies or regulatory actions (policies) and selecting among them. "This selection process necessarily requires the use of value judgments on such issues as the acceptability of risk and the reasonableness of the costs of control" (National Research Council, 1983). Thus the ultimate goal of risk management is to evaluate trade-offs: risk versus economic, political or social consequences.

The risk to public health caused by nitrate contamination of groundwater may be expressed as the risk cost corresponding to event A as an expected value:

$$\text{Risk (A)} = d_0 \int_{-\infty}^{+\infty} [\text{Re}(k(x))g(x)] dx MV \quad [19]$$

- where x = the nitrate level, taken as a random variable,
 $g(x)$ = the probability density function (pdf) of x ,
 $R(k(x))$ = response function value based on animal experiments, that is, given an exposure x , the probability of event A, say a gastric cancer, developing.
 d_0 = the "safe" dose (safe exposure) pertaining to a low probability response value, say $P(A|d_0) = 10^{-6}$ representing background risk.
 $k(x)$ = a safety function, usually kx where $k < 1$ is the safety factor for relating animal to human response.
 M = the mortality rate given event A.
 V = the economic value of human life.

Equation 19 can be used in cases where a single-value function such as the value of human life can be postulated (Graham and Vaupé 1981, Sharefkin et al. 1985). Often there is no such single-value function to express the overall consequence of exposure, in which case multicriterion decision making (MCDM) may be necessary to quantify trade-offs (Haimes and Stakhiv 1986). There are other important uncertainties in expression 19 namely,

- (1) $g(x)$ reflects stochastic uncertainty both in time and space; however, a frequency-base may be available to estimate $g(x)$, and a Bayesian approach can be used to account for small sample size;

- (2) in the high dose region, points on the $R(k(x))$ curve may correspond to frequencies, but the low dose extrapolation is highly subjective.
- (3) the mortality rate can be frequency-based;
- (4) the safety function, the value of human life and the number of people affected must often be determined subjectively.

As a consequence of these imprecise elements, a "classical" risk formulation has two major deficiencies:

- (1) it forces the use of classical probabilities where there is no frequency basis to estimate probabilities (say, in the low-dose response region);
- (2) it uses a single index to account for other uncertain elements, such as a safety factor.

The result of these deficiencies is that the calculated risk cost using equation 19 is far from being reproducible and may not provide a basis for realistic risk assessment or management.

As a consequence of these uncertainties, most risk analyses consider either of two specific cases:

- (1) risk is estimated without considering the consequence; engineering risk is often defined in this way;
- (2) the consequence of exposure is defined as risk without considering the probability of exposure; health risk is often defined this way.

Although it is recognized that both elements are important for a complete description of a groundwater system, here we focus on the exposure and the probability of exposure; that is, as an engineering risk defined as

$$\text{Risk} = P(x > x_0) \quad [20]$$

where x_0 is a threshold nitrate level, typically, regulatory limit.

Contaminant Transport

Bogardi et al. (1986) presented a simulation methodology for estimating the probability density function of a nitrate level x . The nitrate level in ground water was considered to be controlled by three different stochastic inputs: Im meteorology, Is unsaturated soil zone properties and T aquifer properties.

Two of the input elements, Is and T, are stochastic in space, and the question arises as to how areal outputs, in this case areal nitrate levels, can be calculated to account for the spatially random character of the soil parameters. Geostatistics (i.e., the statistics of spatially-correlated random variables) is one approach that has been used successfully to describe the spatial variability of soil parameters (Russo and Bresler 1981; Bogardi et al. 1983). The meteorological elements in the input vector Im exhibit stochasticity both in time and space.

Further research is needed to define a methodology for a simultaneous space-time modeling of all input. The unsaturated zone processes can be represented using an event-based formulation (Bogardi and Bardossy 1984) amenable to an event-based stochastic analysis. To illustrate the methodology, an event-based model for precipitation input is briefly outlined. In event-based modeling, the first step is to define an event. This could simply be the occurrence of daily precipitation amounts exceeding a specified threshold level.

Event-based models may be characterized by two classes of random variables and their probability distribution functions. First, there is the number of events per unit of time (eg., monthly, season, year) or as an alternative, the interarrival time between events (defined here as the time between the beginning of an event and the start of the next event). The second set of random variables describes the events, such as the amount of precipitation, the duration, or the maximum 15-min intensity.

As an example, precipitation during the summer months in semiarid areas is generally of the convective storm type, so that precipitation events appear to occur in an independent manner in time and space and are of very short duration with respect to dry periods. Both empirical and statistical evidence strongly suggest that the number of events, j , per season can be described by a Poisson probability mass function (PMF), $f_N(j)$, written as:

$$f_N(j) = \frac{e^{-m} m^j}{j!} \quad [21]$$

where m is the moment or maximum likelihood estimate given by the mean number of events per season. If the number of events per season is in fact described by a Poisson distribution, then interarrival times T follow an exponential density function (PDF), written as:

$$f_T(t) = u e^{-ut} \quad [22]$$

where the parameter u can be estimated as the mean interarrival time. Inasmuch as the occurrence of summer storms is seldom a pure Poisson process, the distribution of interarrival times may sometimes be described by a gamma (or negative binomial) distribution rather than an exponential (or geometric) distribution.

Under the hypotheses that the occurrence of a thunderstorm and the maximum depth of rainfall within that storm are independent variables, a geometric distribution for point rainfall depths can be derived. Under the same conditions, it can be shown that the distribution for mean areal rainfall could be described by a negative binomial PMF. Analysis of precipitation data suggests that the two-parameter J-shaped gamma PDF, a continuous version of the negative binomial PMF, may provide a better fit to rainfall amounts per event than the derived geometric distribution, this is especially important for a proper fitting of the tail of the distribution.

Using stochastic input, nitrate leaching as a random variable can be calculated. As an alternative to closed form solutions to obtain the PDF of nitrate leaching, Monte Carlo simulation can be used to generate unordered combinations of events occurring during a given season or year. From synthetic rainfall data, a transformed series of seasonal nitrogen leaching amounts can be obtained.

To illustrate the effect of a stochastic rainfall input on nitrogen leaching, a simple numerical example is taken from Bogardi and Bardossy (1984). Over an agricultural area of 1350 ha the soil profile consists of four layers (described by the following depths and conductivities: 0-30 cm, $k=5$ mm/h; 30-45 cm, $k=2.5$ mm/h; 45-75 cm, $k=4.2$ mm/h; 75-250 cm, $k=6.3$ mm/h) above a water table at a depth of 250 cm. Initial nitrogen values are: dissolved nitrogen on soil surface=0.3 kg/ha, soil-bound nitrogen=0.53 g/kg, nitrate in the root zone=78 kg/ha, potentially mineralizable nitrogen=117 kg/ha. As an illustration, results for the month of March are given. Statistics for March precipitation are: mean interarrival time: 3.62 days; depth of events: mean=6.31 mm, standard deviation (s.d.)=7.89 mm; duration: mean=8.22 hours, s.d.=7.5 hours. The initial soil moisture state corresponds approximately to field capacity for all layers. The number of simulations is 100. Two applications of fertilizer are considered:

<u>Case</u>	<u>Date</u>	<u>Amount, kg/ha</u>
a)	30 March	100
b)	15 March	100

Simulated nitrogen leaching amounts are:

<u>Case</u>	<u>Mean, kg/ha</u>	<u>S.D.</u>
a)	0.83	0.60
b)	1.65	1.20

This example demonstrates quantitatively two known facts:

- (1) the timing of fertilizer applications strongly influences the amount of leaching;
- (2) the stochastic character of precipitation causes considerable variance from the mean leaching. Thus, models with a deterministic rainfall input may not be adequate for real-life forecasting and planning.

CONCLUSIONS

Modeling of groundwater pollution due to nonpoint sources is still in its infancy. There are a number of models that are available and could be used. These range from the simple budget models to complex three-dimensional structural models. Simple cell models have been used in Europe, particularly in England and France. A case history from The Netherlands describes the use of a coupled structural model which includes denitrification and in which the aquifer is modeled in three dimensions.

The objective of a structural model is to provide a physically valid representation of the relevant physical and chemical processes that act on a contaminant during its migration through a groundwater system. These processes include advection along groundwater flow paths, hydrodynamic dispersion, diffusion, adsorption, and chemical and biochemical reactions. All of these processes may vary along migration paths.

Since the physical and geochemical parameters driving these processes are often poorly known, structural models are used to best advantage in sensitivity analyses in which the uncertain parameters are varied within certain ranges and the corresponding response of the model is observed. A model used in this way can provide valuable insight into the possible fate of contaminants. Structural models are also useful in assessing the implications of worst-case contamination scenarios, or the merits of different management schemes. In that sense, models play not only a predictive, but also an educational role.

Advective-dispersive models for sand and gravel aquifers incorporating simple chemical reactions have been developed and can be considered as mature, at least in two dimensions. Advances in stochastic methods made in the last few years now provide a rational basis for dealing with uncertainties in the structure of heterogeneous media, and for the definition of the dispersion parameters. Advective-diffusive models that recognize the diffusive interaction between mobile and stagnant zones, and that are applicable to systems with strong permeability contrasts such as sand-clay systems, have also been developed.

For more complex geochemical or biochemical processes, geochemical equilibrium or kinetic models are available. The coupling of general geochemical models with dynamic transport models, which multiplies the complexities inherent in each of these models, however still remains as a major challenge to researchers. Some pioneering papers have appeared in the literature, and the future will undoubtedly see increasing activity in this area.

The case history from The Netherlands shows that current modeling modules can be combined to model nonpoint-source pollution. The results are presented at a scale at which management decisions can be made. A clear advantage of the modeling approach is that the influence of factors such as the depth at which withdrawals are made can be evaluated. Also the importance of such factors as the decomposition rate of organic matter can be demonstrated.

Risk is an element that eventually must be considered in relation to cost. Prediction of risk must account for the uncertainties in aquifer properties and the stochastic nature of the various inputs. A methodological framework is outlined and a simple example shows how these uncertainties affect results. Realistic modeling considering risk and uncertainty using the structural approach described for the Netherlands is beyond today's computers.

As a general conclusion, we wish to emphasize that the control of nonpoint-source agricultural pollution implies decisions that can be ordered by a careful use of a combination of models, usually starting with budget and reservoir models and eventually involving structural models, and the concepts of risk and uncertainty.

ACKNOWLEDGEMENTS

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A REVIEW OF GROUNDWATER MODELS FOR ASSESSMENT AND PREDICTION OF NONPOINT-SOURCE POLLUTION

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ABSTRACT

Various approaches to nonpoint-source contamination in saturated groundwater flow from very simple lumped models to complex models describing flow, transport, and chemical reactions in heterogeneous groundwater systems are examined.

INTRODUCTION

Currently, nonpoint-source pollution is a major challenge for agriculture, and certainly ranks as a factor in environmental degradation of groundwater and streams in the United States. From a scientific perspective, the analysis and prediction of diffuse sources of groundwater contamination have been hampered because of several interrelated factors: the large scale of the problem; the difficulty of sampling and characterizing the "diffuse source"; and an incomplete understanding of fluid flow and chemical transport in large scale environmental systems. The issue of scale is, in our opinion, fundamental to the problem of nonpoint-source pollution. Recent advances have been made with regard to the so-called "scale effect" for point sources (Gelhar and Axness 1983), however, little attention is being given to an encompassing theory for distributed sources. Experiments relating to the scale issue for point sources have gone from laboratory tracer studies to intermediate scale (1-100 meters) field experiments (Freyberg 1986). Nonpoint sources, operating at a scale of motion which we might call the "aquifer" or "watershed" scale, are only beginning to receive this same scientific attention.

The difficulty in sampling and characterizing nonpoint sources is an issue related to the problem of scale. Even where uniformly applied, it has been shown that tracers move through soils to groundwater at remarkably different rates. Considering the time variations of precipitation and evaporation which effectively drive contaminant motion, the impact of space-time variability on modeling and prediction cannot be neglected. Finally, modeling complex geochemical processes, coupled with the physical processes of subsurface flow and transport, will be essential to understanding the evolution and retention of nonpoint-source chemicals in the subsurface.

The problem of environmental management of nonpoint-source pollution requires the best available answers. There is no doubt that mathematical models will play an important role in this effort. In the present paper we review a range of approaches to the general problem of modeling and the prediction of nonpoint-source contaminants in groundwater. We make no attempt to provide a comprehensive review, but direct our efforts toward past approaches and possible directions for future research.

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APPROACHES TO MODELING NONPOINT-SOURCE CONTAMINANT TRANSPORT

A broad range of mathematical approaches to the question of nonpoint-source pollution have been proposed in the literature. In this summary we will cover four general approaches or classes of problems: the probabilistic approach, the input-output or systems approach, the multi-dimensional distributed model approach, and the coupled transport and reaction modeling approach.

Probability Models For "Age" and "Transit Time" Distributions

One basic approach to environmental transport of chemicals in the subsurface is based on the determination of the transit time and age distribution of dissolved solutes using the probability theory (Eriksson 1971; Jury et al. 1986); Bolin and Rodhe (1973) illustrate the method. For an arbitrary reservoir, a simple relation exists between the probability density function (pdf) for the "age" of elements within the reservoir $\psi(\tau)$, and the pdf for the "transit time" of elements as they exit the reservoir $\phi(\tau)$. For a steady-state system which exchanges mass with other external and undefined reservoirs, each element of mass is characterized by the time, τ , that has elapsed since the element entered the reservoir, where τ is the age of the element. The probability distribution for the mass is determined by cumulatively ordering each element of the reservoir to produce the cumulative mass function $M(\tau)$, where $M_0 = M(\infty)$ is the total mass in the reservoir. The normalized distribution $M(\tau)/M_0$ is related to the mass or "age" density for the reservoir $\psi(\tau)$ by the following relationship:

$$\psi(\tau) = \frac{d(M/M_0)}{d\tau} \text{ or } \frac{M(\tau)}{M_0} = \int_0^\tau \psi(\xi) d\xi, \quad [1]$$

where ψ has the usual properties of a probability density. The transit time through the system is also described by a cumulative function $F(\tau)$, defined as the mass flux from the reservoir for elements which have spent a time $t \leq \tau$ in the reservoir. The "transit time" or "flux density" of the reservoir $\phi(\tau)$ is defined as:

$$\phi(\tau) = \frac{d(F/F_0)}{d\tau} \text{ or } \frac{F(\tau)}{F_0} = \int_0^\tau \phi(\tau) d\tau, \quad [2]$$

where F_0 is the steady-state flux through the reservoir. Bolin and Rodhe (1973) show that a unique relationship exists between the age and transit time densities, namely:

$$\phi(\tau) = - \frac{M_0}{F_0} \frac{d\psi}{d\tau}. \quad [3]$$

The first moment of the transit time distribution $\phi(\tau)$ is the residence time τ_0 defined by:

$$\tau_0 = \int_0^\infty \tau \phi(\tau) d\tau = \frac{M_0}{F_0}. \quad [4]$$

The mean age of the reservoir τ_a , can be determined from the first moment of the age density $\psi(\tau)$

$$\tau_a = \int_0^\infty \tau \psi(\tau) d\tau. \quad [5]$$

This approach for nonpoint-source pollution is attractive because if one were able to know either the age density $\psi(\tau)$ or transit time density $\phi(\tau)$ from physical arguments, then one could use the properties of the known density to derive the other, and in addition, construct all its moments. The difficulty, of course, is in determining the appropriate probability model. An interesting special case occurs when $\tau_a = \tau_0$, where $\psi(\tau) = \phi(\tau)$ (see Bolin and Rodhe 1973). The common density function turns out to be the exponential (fig. 1):

$$\begin{aligned}\phi(\tau) = \psi(\tau) &= \frac{1}{\tau_0} \exp \left\{ -\frac{\tau}{\tau_0} \right\} & ; \quad \tau \geq 0 \\ &= 0 & ; \quad \tau < 0.\end{aligned}\tag{6}$$

Exponential densities characterize the flux from reservoirs in which elements have a constant probability of being removed per unit time, such as radioactive decay and first order chemical reactions. Input/output systems with exponential densities are termed "well mixed," or the solute mass in the reservoir is proportional to the outflow mass flux. Bolin and Rodhe (1973) point out that geophysical reservoirs of this type (the atmosphere, lakes, oceans, aquifers, etc.) can generally be characterized as having a large source area and a sink region which is isolated or limited in size. For this reason, these systems have appeal for the nonpoint-source problem where the source is areally distributed and outflow occurs at a stream or well.

The difficulty with the probability-based development given here is that no consideration is given to the particular aquifer geometry and the physics of the flow system, or to transients in the input source.

A Linear Reservoir Model For Transient Input-Output Systems

With nonpoint-source pollution one is often concerned with the effect of the contaminant at points or zones of flow convergence, such as discharge from a pumping well, baseflow to a stream, or the effluent of an agricultural drain. Nonpoint sources have the greatest potential for human or biological exposure at these locations. Where the internal characteristics of the groundwater system are largely undefined, the linear reservoir or lumped-parameter model has been shown to be a practical approach to modeling input/output dynamics for nonpoint-source pollution (Gelhar and Wilson 1974). For the setting illustrated in figure 2, the model equation is given by:

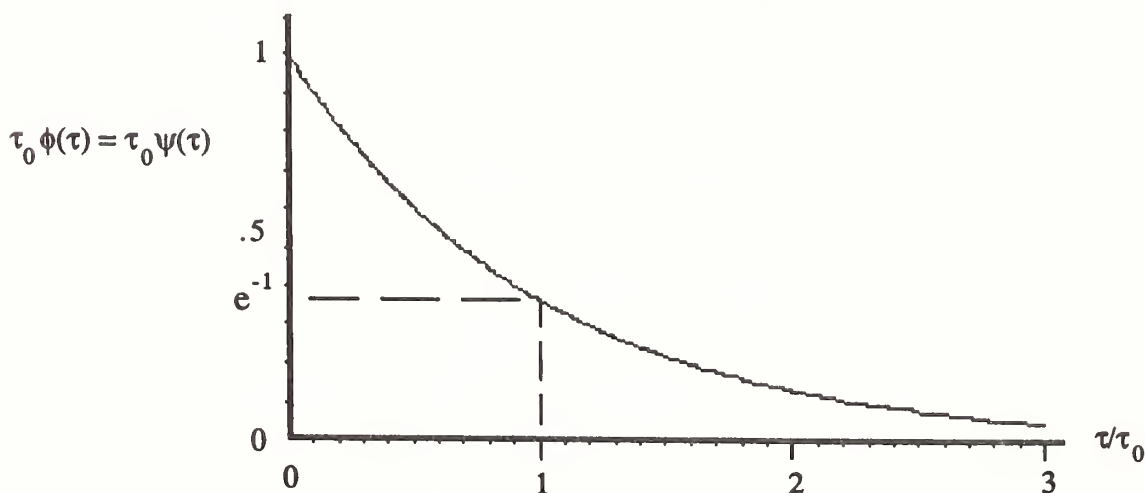


Figure 1.
Exponential probability density for the average age of elements of the system, $\psi(\tau)$, and the average transit time or residence time of elements leaving the system, $\phi(\tau)$.

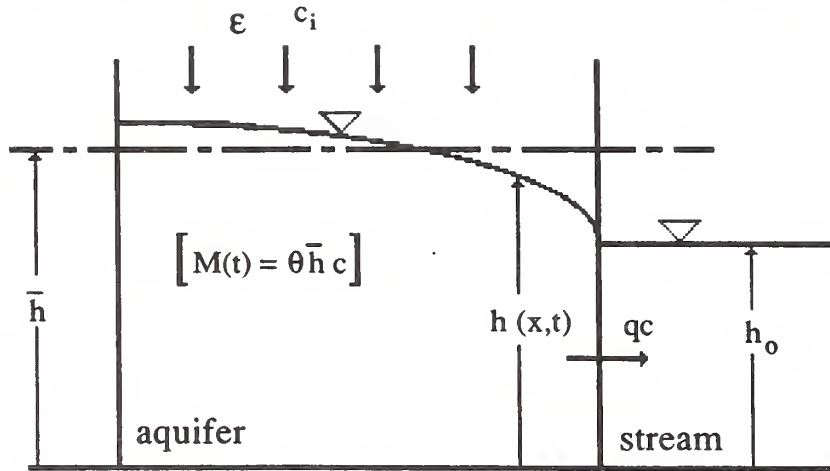


Figure 2.
A linear reservoir representation for nonpoint-source contamination of concentration $c_i(t)$, where $M(t)$ is the solute mass averaged over the surface area of the aquifer.

$$\frac{dM}{dt} = F_i - F \pm F_s, \quad [7]$$

where the variables are normalized by the aquifer area:

$$\begin{aligned} M &= \text{spatial average mass of solute in the aquifer/unit area [M/L}^2\text{]}, \\ F_i &= \epsilon c_i, \text{ source mass flux of concentration } c_i(t)/\text{unit area [M/L}^2\text{T]}, \\ F &= qc, \text{ outflow mass flux of concentration } c(t)/\text{unit area [M/L}^2\text{T]}, \\ F_s &= \text{other sources or sinks for the solute/unit area [M/L}^2\text{T]}, \\ q &= \text{outflow/unit area [L/T], and} \\ \epsilon &= \text{inflow or recharge [L/T]}. \end{aligned}$$

The approach assumes that the mass of solute of concentration $c(t)$ in the aquifer is represented by its spatial average:

$$M_v(t) = \theta \int_{V(x,y,z)} c(x,y,z,t) dV. \quad [8]$$

For thin aquifers, the mass per unit aquifer surface area is approximated as:

$$M(t) = \theta \bar{h}(t) c(t), \quad [9]$$

where \bar{q} = the porosity and
 $\bar{h}(t)$ = the mean saturated thickness.

For steady flow ($q = \epsilon$, $h = \text{constant}$), the transport equation takes the form

$$\frac{dc}{dt} + \frac{c}{\tau_0} = \frac{c_i}{\tau_0} \pm r', \quad [10]$$

where r' represents other sources and sinks such as sorption or decay, and the characteristic time τ_0 , or residence time, is defined as:

$$\tau_0 = \frac{M}{m} = \frac{\text{reservoir fluid mass}}{\text{reservoir mass flux}} \sim \frac{\theta \bar{h}}{q} = \frac{\text{fluid volume}}{\text{fluid flux}} \quad [11]$$

assuming the mean aquifer concentration is the same as the outflow concentration

$$\bar{c}_{\text{aquifer}} = c_{\text{outflow}}.$$

A general solution to the model is found via the convolution integral where $g(t)$ is the impulse response function and c_0 is the initial concentration

$$c(t) = C_0 \tau_0 g(t) + \int_0^t g(t-\tau) c_i(\tau) d\tau. \quad [12]$$

For $r' = 0$, $c_0 = 0$, and $c_i = \delta(t)$ the solution has the form

$$c(t) = g(t) = \frac{1}{\tau_0} \exp \left\{ -\frac{t}{\tau_0} \right\} \quad [13]$$

showing that the impulse response function for the linear reservoir or mixing cell model is the exponential function and identical to the previous case based on probability arguments. This input/output characteristics model of nonpoint-source pollution has been applied by a number of authors (van der Molen 1973, Gelhar and Wilson 1974, McLin and Gelhar 1979, Raats 1981, Duffy and Gelhar 1986).

Although the lumped approach may provide a practical approach to the impact of nonpoint sources at a point of outflow, it does not provide information about the spatial pattern of flow or concentration within the aquifer.

Nonpoint Sources In Multidimensional, Distributed Systems

A general approach to modeling nonpoint-source pollution relies on the three-dimensional version of Darcy's law for saturated flow

$$q_i = - \frac{\kappa_{ij}}{\mu} \left[\frac{\partial p}{\partial x_j} + \rho g n_j \right] \quad i, j = 1, 2, 3 \quad [14]$$

where

q_i	=	Darcy velocity [L/T],
κ_{ij}	=	porous medium permeability tensor [L^2],
g	=	gravitational constant [L/T^2],
p	=	fluid pressure [$M/(LT^2)$],
n_i	=	gradient of the elevation head, $\delta z / \delta x_i$ [L/L],
ρ	=	fluid density [M/L^3], and
μ	=	fluid viscosity [$M/(LT)$].

The conservation equation for the bulk fluid, including the effects of natural groundwater inflows, injection or withdrawal wells, and variable fluid density, is given by

$$\frac{\delta}{\delta x_i} \left[\frac{\rho \kappa_{ij}}{\mu} \left[\frac{\delta p}{\delta x_j} + \rho g n_j \right] \right] - \rho (\alpha + \beta \theta) \frac{\delta p}{\delta t} \pm r' , \quad [15]$$

where α = coef. of compressibility of the fluid $[M/LT^2]^{-1}$,
 β = coef. of compressibility of the medium $[M/LT^2]^{-1}$,
 θ = porosity $[L/L]$, and
 r' = fluid source/sink term.

The corresponding solute transport equation can be written as:

$$\frac{\delta}{\delta x_i} \left[\theta \rho D_{ij} \frac{\delta c}{\delta x_j} \right] - \rho q_i \frac{\delta c}{\delta x_i} - \theta \rho \frac{\delta c}{\delta t} \pm r' , \quad [16]$$

where $c(x,y,z,t)$ = concentration $[M/L^3]$,
 r' = solute source/sink,
 D_{ij} = dispersion coef. tensor (Bear, 1972) $[L^2/T]$; and

$$\theta D_{ij} = a_t |q| \delta_{ij} + (a_l - a_t) \frac{q_i q_j}{|q|} + \theta D_0 \delta_{ij} , \quad [17]$$

where D_0 = molecular diffusion coefficient,
 δ_{ij} = identity matrix,
 a_l = longitudinal dispersivities, and
 a_t = transverse dispersivities.

Generally, nonpoint-source contamination enters and leaves the subsurface system through the boundaries of the porous domain. The contaminant source and the attendant fluid flux enter the above equations through specification of boundary conditions of the first (Dirichlet), second (Neumann), or third type (mixed). Specific examples are given later. Analytic solutions of the above system of equations can only be found for very simple porous medium geometries and boundary conditions. Solutions generally require the application of numerical methods such as the finite element or finite difference technique. Details of the computational aspects of the problem can be found in Huyakorn and Pinder (1983) and will not be given here. However, we will later examine simplified numerical results which provide insight into the problem of modeling nonpoint-source pollution.

REACTION MODELS AND MASS TRANSPORT

The treatment of nonpoint sources immediately brings to mind extensive areal domains. Such domains have spatially variable mineralogy; hence, in addition to transport phenomena, reactive geochemistry will contribute to the spatial variability of water quality. However, the natural stratigraphic structure of geologic deposits and the equilibrium character of many geochemistry reactions imply a certain relevance of equilibrium geochemistry models because of the potential for substantial contact time with dominant geologic units. While a hydrologic basin may be modeled for the transport of conservative solute using the lumped parameter methods, the coupled geochemistry and transport models described in the following section rely on a distributed model of mineral and aqueous composition and physical transport mechanisms. Thus, the line of thought introduced in the preceding section is not followed here. Instead, concepts of modeling

that allow one to account for complexities of distributed properties and reactive transport phenomena are described.

Coupled models of multispecies transport originate in both the agricultural literature (Dutt et al. 1972) and the water resources literature (Rubin and James 1973). These models have been developed to account for the interactions among aqueous and sorbed species and complexes under environmental conditions where the physical transport of these components cannot be neglected. Simulation of reactive solute transport in an aquifer can be approached in two ways: simple chemical mass transfer and mechanistic geochemistry (Cherry et al. 1984). The first approach emphasizes the prediction of the advance rate and shape of the solute front. The latter approach emphasizes the prediction of solute concentration within the plume which is caused by aqueous complexation, adsorption/desorption, precipitation/dissolution, and oxidation/reduction.

Incorporation of simple chemical mass transfer, such as sorption, into a transport model is achieved by assuming that the solid phase concentration, s , is a function of the solution phase concentration, c . Commonly applied chemical mass-transfer models include the linear, Freundlich, and Langmuir sorption isotherms. The second approach, based on mechanistic-process and reaction models, has been developed to predict both the form and concentration of aqueous species and solid phases resulting from adsorption and precipitation reactions. Attention is focused on combined geochemistry and transport models employing the second approach.

For mechanistic models, a code is clearly distinguished by the coupling approach adopted. Two distinct approaches have been taken to incorporate mechanistic geochemistry in the simulation of solute transport: the direct approach which uses a simultaneous solution, and a two-step approach which seeks a consistent solution between independently posed and solved chemical equilibrium reactions and solute mass-transport equations.

Carnahan (1987) summarized code complexity for coupled models. An expanded chronology of coupled codes and a summary of their attributes are shown in table 1. Only three of the codes are truly multidimensional, although nearly all of the other codes could be applied to simulate transport along streamtubes defined within multidimensional flow fields. Most of the codes simulate transport from a continuum basis, using either a finite difference or finite element formulation. An analytical model of the transport processes is employed in one code and a mixing cell approach is employed in five codes. Direct and two-step coupling approaches have been used for coupling mechanistic geochemistry with solute transport. Nearly all of the listed codes use a two-step coupling approach. All but one of the codes are based on thermodynamic equilibrium; all but one include some capability to simulate sorption; and roughly half consider precipitation. Presently, there is a clear trend toward using the two-step coupling procedure and incorporating a more complete suite of geochemistry processes (i.e., aqueous speciation, sorption, and precipitation).

Direct Coupling

Rubin (1983) outlined a general mathematical framework for the direct approach. Rubin and James (1973) first presented a finite element model of transport and direct coupling. The geochemistry submodels appear as explicit terms in the transport equations. The static mass balance equations, the basis of an equilibrium geochemistry model, are replaced by the dynamic solute transport equations. Rubin and James (1973) examined several hypothetical cases involving exchange in binary and ternary systems, and binary exchange influenced by the precipitation/dissolution of gypsum. Valocchi et al. (1981) extended the approach of Rubin and James by examining homovalent and heterovalent exchange in binary and ternary systems of one and two spatial dimensions.

Table 1.
Summary of computer programs coupling mechanistic models of transport
and geochemistry.

<u>Authors/Attributes</u>	<u>Dim.</u>	<u>Num. Tech.¹</u>	<u>Coupling Method</u>	<u>AquSpec</u>	<u>Chemistry Model</u>			
					<u>Sorpt.²</u>	<u>Precip</u>	<u>Act. Coef.³</u>	<u>Chem.</u>
Dutt et al. 1972	1	FD	2-step	no	IE	yes	D-H	equil
Rubin & James '73	1	FE	direct	no	IE	yes	no	equil
Grove & Wood '79	1	FD	2-step	yes	IE	yes	D-H	equil
Valocchi et al. 1981	2	FE	direct	no	IE	no	no	equil
Reardon 1981	1	MC	2-step	no	IE	yes	no	equil
Jennings et al. 1982	1	FE	direct	yes	SC,L	no	no	equil
Dance & Reardon 1983	1	MC	2-step	no	IE	yes	no	equil
Miller & Benson 1983	1	FD	direct	yes	IE,SC	no	Davies	equil
Miller 1983	1	FD	direct	yes	IE,SC	yes	Davies	equil
Schulz & Reardon 1983	2	Analyt.	2-step	no	IE	yes	no	equil
Kirkner et al. 1984	1	FE	2-step	yes	IE	no	no	equil
Morrey & Hostetler 1985	1	MC- Markov	2-step	yes	IE,SC	yes	Davies & D-H	equil
van Ommen '85	1	MC	2-step	no	IE	no	Davies	equil
Cederburg '85 & Cederburg et al. 1985	1	FE	2-step	yes	SC	no	no	equil
Kirkner et al. 1985	1	FE	2-step	yes	L	no	no	kinetic
Narasimhan et al. 1986	2	IFD	2-step	yes	no	yes	Davies	equil
Carnahan '85'86	1	FD	direct	yes	no	yes	Davies	equil
Appelo & Willemssen 1987	1	MC	2-step	yes	IE	no	D-H	equil

¹ MC=mixing cell, FE=finite element, FD=finite difference, IFD=integrated finite difference

² IE=ion exchange, SC=surface complexation, L=Langmuir

³ D-H=Debye-Huckel

Using a two-dimensional Galerkin finite-element model of transport, they presented what has become a classic benchmark and validation problem for coupled models: the injection of treated municipal effluent into a leaky confined aquifer in the Palo Alto Baylands region of California. Jennings et al. (1982) incorporated soluble complexation and competitive (Langmuir type) sorption in a one-dimensional transport model. Each of the above models retains concentration as the dependent variable rather than correcting for activity. Later models (Miller and Benson 1983, Miller 1983, Carnahan 1986) make this correction using the Davies model. Miller and Benson (1983) developed the CHEMTRN model that extended the direct coupled formulation to include aqueous speciation, multicomponent sorption, and dissociation of water. The CHEMTRN model is categorized as a direct approach because it obtains a simultaneous solution to both the transport and geochemistry problems. However, instead of incorporating geochemical reactions directly into the transport equations, the geochemical and transport equations are formulated as an overall equation set and are solved simultaneously. Miller (1983) extended this model to include precipitation and dissolution.

Recently, Willis and Rubin (1987) and Bahr and Rubin (1987) presented detailed studies of specific cases which arise in Rubin's (1983) framework of mathematical formulations. They presented and analyzed formulations which involve moving dissolution boundaries and kinetic versus local equilibrium assumptions in the presence of surface reactions.

Two-Step Coupling

The two-step approach results in a sequential solution of algebraic equations describing equilibrium chemistry, and partial differential equations describing mass transport. Dutt et al. (1972) developed a coupled model of transient flow and transport in the vadose zone for nitrogen transformations and uptake by crops in the presence of gypsum and lime. Ion exchange models were used to simulate calcium-sodium, calcium-magnesium, and sodium-ammonia exchanges. The model approximated dispersion as simple mixing within cells associated with nodes of the finite-difference flow model. The time step of the model is a function of the highest water flux rate in the soil column; thus nodes that exhibit high water flux rates are given less opportunity to disperse than those with lower rates. Physically, the model adequately simulated convective transport along streamtubes, while the mixing cell approach to dispersion was less satisfactory.

Grove and Wood (1979) coupled one-dimensional transport with mineral precipitation/dissolution and ion exchange reactions. This model included some activity corrections; however, no attempt was made to provide a mass balance for water. Patterned after the model of Dutt et al. (1972), Grove and Wood included an explicit model of dispersion in their finite-difference model of transport. The model was used to study water quality changes resulting from the artificial recharge of an aquifer.

Kirkner et al. (1984) present a one-dimensional finite-element transport model with a geochemistry model of sorption and soluble complexation. A version of this model, FIESTA, included a general simulation of aqueous speciation by incorporating the geochemistry code MINEQL (Westall et al. 1976). As in the Grove and Wood model, no explicit mass balance was kept of water and no activity corrections were made for water; hence, the model is applicable to dilute solutions only. Previous models had included transport equations for each chemical species. Kirkner et al. (1984) formulated the transport equations only for chemical components, thus achieving a substantial economy. Others, particularly Cederberg (1985), also recognized and incorporated this economy in two-step coupled models. In addition, Kirkner et al. (1985) presented a two-step model incorporating kinetic considerations in solid-phase chemical interactions.

The two-step approach has also been used to address multidimensional transport phenomena. Schulz and Reardon (1983) created a two-dimensional mixing-cell/analytical model that includes

geochemical reactions of mineral precipitation/dissolution and ion exchange. This particular model also includes transverse dispersion, but it is only applicable to unidirectional groundwater flows. It has limited applicability to realistic aquifer settings where arbitrarily-oriented surfaces and flow fields are of interest. Cederberg et al. (1985) presented the TRANQL model which employs the geochemical module MICROQL (Westall 1979) and reactions for sorption, complexation, dissociation of water, and ion exchange. The MICROQL module is a smaller version of the more comprehensive MINEQL code (Westall et al. 1976). TRANQL employs a finite element model of solute migration and is exercised on one-dimensional and axisymmetric radial flow cases. This model could be extended to address arbitrary two-dimensional systems. Narasimhan et al. (1986) developed a dynamic mixing model, DYNAMIX. It addresses two-dimensional domains by simulating transport with an integrated finite difference model; however, the coupled calculations are performed in one dimension. Geochemistry is simulated with a variable pH, speciation-complexation model that includes mineral precipitation and dissolution.

The equilibrium geochemistry code PHREEQE (Parkhurst et al. 1980) is used in the DYNAMIX code. Elemental volumes, e.g., cells of the integrated finite difference grid, are interpreted as mixing cells for the geochemistry model in this formulation. The method employed in DYNAMIX performs transport mass balance on cells (which surround nodes) by explicitly calculating mass crossing boundaries between cells. This method of simulating transport may have better mass conservation characteristics at the local or individual cell level than other continuum methods (e.g., finite-element and standard finite-difference methods).

Reardon (1981) used a mixing-cell model of transport and geochemistry to explore the relevance of the linear sorption isotherm or distribution coefficient model. A simple mixing-cell model was used to demonstrate the dynamic character of solute migration resulting from geochemical processes of ion exchange, calcite dissolution, and aqueous speciation of carbonate, bicarbonate, and sulfate ion pairs of Ca, Mg, Na, and K. Because he did not intend to simulate realistic transport processes, Reardon did not simulate the dispersive transport process. Dance and Reardon (1983) incorporated a dispersion-diffusion process submodel in a one-dimensional mixing-cell model. Dispersion-diffusion was simulated by permitting a fraction of the solute mass to move one cell upgradient and one cell downgradient from an originating cell. Such a model creates what is essentially a three-cell distribution approximating a Gaussian distribution of dispersion and diffusion. Advection is simulated by moving the solute mass one cell downgradient. Thus, the net transport process does not permit any upgradient migration of solute. Schulz and Reardon (1983) extended this approach to include transverse dispersion; however, their use of an analytical model of dispersive phenomena limits the applicability of the model to one-dimensional flow fields.

Van Ommen (1985) derived a relationship between the dispersion coefficient of the classical convection-dispersion equation and the time step and cell size of a simple mixing-cell model. Numerical dispersion of the mixing cell method is essentially thought to mimic physical dispersion. Two cases of ion-exchange reactions were used by van Ommen to test his model: sodium exchange with a complex initially occupied with calcium, and calcium exchange with a complex initially occupied with sodium. Ion exchange was modeled with the Gapon and Kerr equations, and the Davies equation is used to calculate activity coefficients.

Appelo and Willemssen (1987) derived a formal relationship between the mixing factor of the Dance and Reardon (1983) model and the dispersion coefficient of the classical convection-dispersion equation. This model of a three-cell dispersion-diffusion distribution exhibits increased accuracy with advanced time steps, e.g., 10% error after 3 time steps, 5% error after 10 time steps, and negligible error after 40 time steps. The geochemistry module of the Appelo and Willemssen model is the EQ3/6 model of Wolery (1982).

Morrey and Hostetler (1985) developed a one-dimensional mixing-cell model based on a Markov transport algorithm. The Markov algorithm (Morrey et al. 1988), based on a probability density function (pdf) representation of longitudinal dispersive transport, can employ either a Gaussian or lognormal pdf. The pdf describes the distribution about the mean caused by the dispersion and diffusion processes. The Markov transformation matrix accounts for both the pdf distribution and the translation resulting from the mean pore-water velocity. The geochemistry module of their code is designed to be comprehensive in its simulation of geochemical reactions and includes aqueous speciation, surface complexation, ion exchange, and precipitation.

OBSERVATIONS, EXPERIMENTS, AND APPLICATIONS

A range of experimental and numerical results are examined to shed some light on the practical problem of modeling nonpoint-source contamination in the field. No attempt is made to review the general literature on this extensive subject.

Field Evidence For An Integrated Volume-Flux Relation

Some experimental results from an agricultural drainage system in New Mexico suggest that spatial integration holds some promise as a simplified physical approach to nonpoint-source transport. This idea which, to our knowledge, was first proposed by Kraijenhoff van de Leur (1958), states that the integrated aquifer fluid volume is proportional to baseflow or flux from the reservoir. For thin aquifers or drainage systems, the integrated volume is constructed by averaging the saturated thickness from known observation wells. Gelhar and Wilson (1974) proposed a volume-flux relation of the form

$$q = a(\bar{h} - h_0) \quad [18]$$

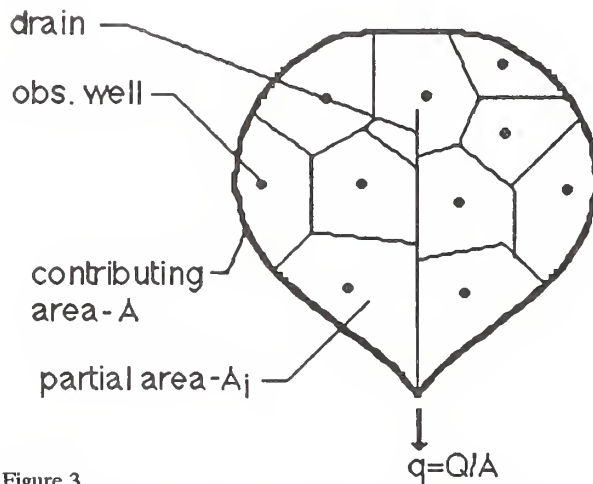
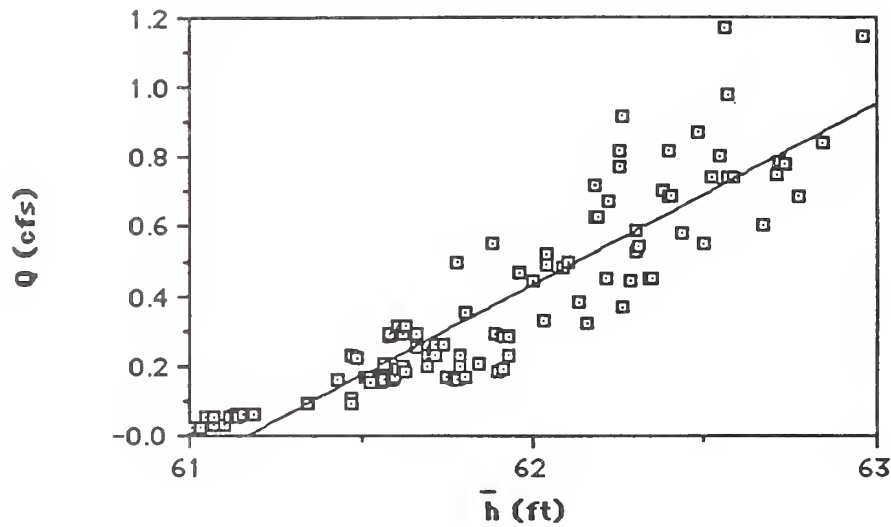
which provides an integrated equivalent to Darcy's law where the flux is proportional to either potential energy or excess hydraulic head. Wierenga et al. (1981) examined the volume-flux relation for an irrigated drainage system in New Mexico, and the results are shown in figure 3. In this example, the areal-average water level is plotted against total drainflow. For high flows a linear relation is evident; however, a distinct nonlinear result is evident for low flow periods. At present there has been no physical explanation of the nonlinear behavior, but it seems likely that it is related to a shrinking of the contributing area to the drain during low flows.

For a nonpoint contaminant, it was shown that the residence time, τ_0 , is the coefficient of proportionality between the integrated fluid volume and the net fluid flux from the aquifer. Under these conditions, a mixing cell or linear reservoir model is a useful approximation for input/output contaminant behavior, and the approach offers a physical basis for the application of lumped models to nonpoint-source contamination.

Numerical Experiments For 2-D Flow In A Dispersive System

Although the above example provides a useful relation for the integrated volume and flux of the system, the result tells us little about how local advective-dispersive processes might affect outflow concentration in the aquifer. The first author and several graduate students have examined the role of dispersive mixing through a series of numerical experiments (Duffy 1985, and Lee M.S. thesis USU 1988). A sample of these results is presented in the simplified aquifer-drain geometry of figure 4 for the problem of diffuse contamination. The porous medium of thickness D and length L is assumed to be homogeneous and isotropic with respect to permeability and porosity. A nonpoint source of contamination of concentration c_0 and infiltration flux rate ϵ is applied uniformly across the upper surface. The sides are specified as "no flux" boundaries with respect to the fluid and the contaminant. The upper flux boundary condition is a reasonable physical

Integrated Volume-Discharge



$$\bar{h}(t) = \sum_i \frac{A}{A_i} h_i(t)$$

= weighted mean
saturated thickness

Figure 3.
Relation between area-weighted-mean aquifer volume and the baseflow
and/or drainage for a small-scale drainage system at San Acacia,
New Mexico (data from Wierenga et al. 1981).

approximation as long as the infiltration rate is much smaller than the mean hydraulic conductivity of the medium, and the maximum change in hydraulic head is small relative to the saturated thickness, say $\Delta h/D \leq 0.1$. The steady-state outflow per unit length of drain is $Q = \varepsilon L$, where r_0 is the radius of the drain:

$$r_0 = (x_0^2 + y_0^2)^{1/2}.$$

The initial concentration in the aquifer is specified as c_i . The flow and transport equations were nondimensionalized by the characteristic length, velocity, and time L , K , and t_0 , respectively, leading to the dimensionless variables

$$x_i^* = \frac{x_i}{L}, \quad t^* = \frac{Kt}{L}, \quad q_i^* = \frac{q_i}{K}, \quad \varepsilon^* = \frac{\varepsilon}{K}, \quad c^* = \frac{c}{c_0}, \quad h^* = \frac{h}{L} \quad [19]$$

and parameters

$$K^* = \frac{K}{K}, D_{ij}^* = \frac{D_{ij}}{KL}, D_0^* = \frac{D_{ij}}{KL}, a_i^* = \frac{a_i}{L}, \text{ and } a_t^* = \frac{a_t}{L}. \quad [20]$$

The resulting form of the flow and transport equation is given by

$$\frac{\delta q_i^*}{\delta x_i^*} = 0 \quad [21]$$

$$\theta \frac{\delta c^*}{\delta t^*} = \frac{\delta}{\delta x_i^*} \theta D_{ij}^* \frac{\delta c^*}{\delta x_i^*} - q_i^* \frac{\delta c^*}{\delta x_i^*} \quad i, j = 1, 2. \quad [22]$$

The above system of partial differential equations were solved numerically using the finite element code SUTRA (Voss 1984), for the case of an initially contaminated aquifer, with uniform concentration $c_i^* = 1$ and flushed by infiltration to the aquifer with concentration $c^* = 0$. One of the reasons for conducting numerical experiments of this sort was to determine the effect of dispersive mixing on the outflow concentration for this system. Figure 5 provides an example of the distributed model response for a range of dispersivity ratios. Also plotted on the figure is the mixing cell result. The first observation is that there is almost no difference between the lumped and distributed results for the idealized case of uniform aquifer properties. This was the case for all values of dispersivity chosen. The conclusion from the numerical experiments was that dispersive mixing has little effect on the overall system response and, as has been pointed out by Eldor and Dagan (1972) and McLin (1979), that the nonpoint-source problem is dominated by convection.

These and other simulations by Lee (1988), where the hydraulic conductivity is simulated as a random field, have shown that the role dispersive mixing plays in the prediction of nonpoint sources depends on the scale of observation. On a local scale, such as a soil profile or along a particular flow path in an aquifer, it is certain that dispersive mixing is critical to prediction. However, for situations where the measured solute concentration is integrated (such as at

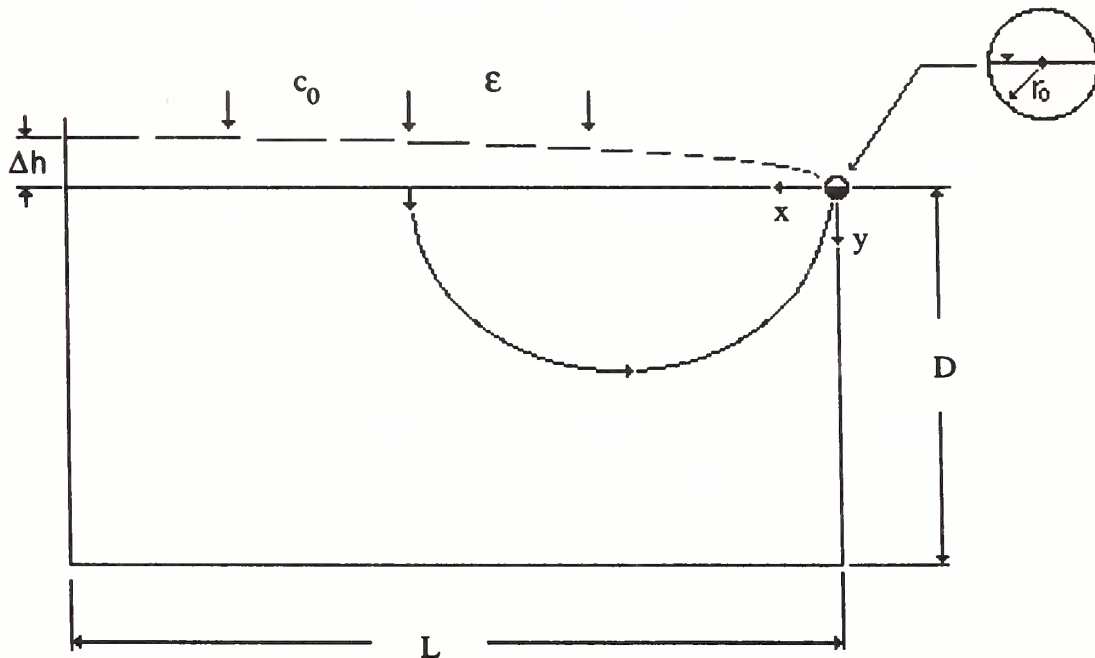


Figure 4.
A simple geometry for a nonpoint source of concentration c_i , and flow convergence at a drain.

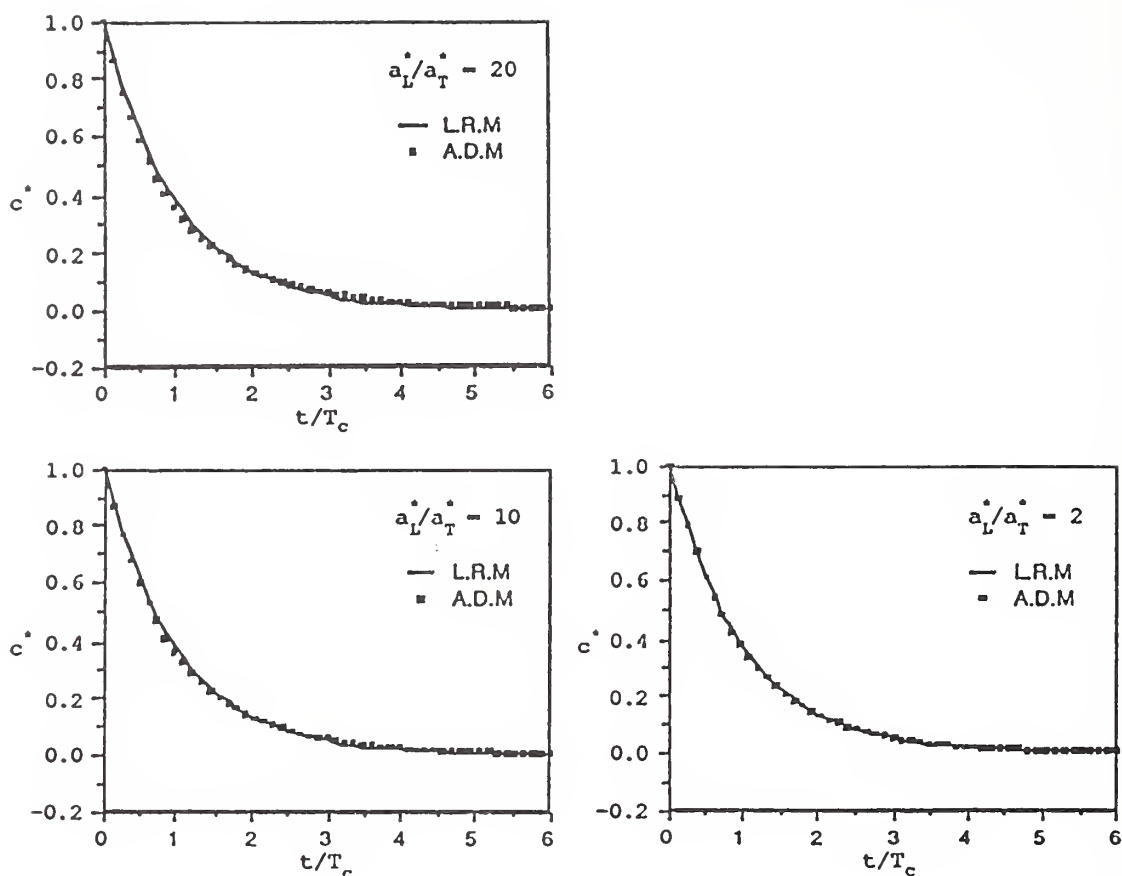


Figure 5.
Dimensionless outflow concentration for the convection-dispersion model (C.D.M) evaluated at r_0 versus dimensionless time ($T_c = \tau_0$ = residence time), compared with the linear reservoir model (L.R.M) (after D.H. Lee 1988). The result demonstrates the insensitivity of the outflow concentration to dispersion.

apumping well, agricultural drain, or a stream) the predicted concentration shows no sensitivity to dispersive attenuation. In this case much simpler transport models may be applicable. By simplifying transport equations from a physical basis (integration) rather than a "black box" approach, the analysis of complex geochemical and biological interaction becomes a more realistic proposition.

Simulation Of Aldicarb Source Variation On Long Island

The nature of groundwater contamination resulting from agricultural use of pesticides is characterized by highly transient loadings with rainfall events dominating the timing and magnitude of the pesticide loads and leaching below the root zone. The fate of dissolved pollutants, including their transport through the vadose zone, is governed not only by vertical infiltration, but also by sorption and biodegradation processes. Thus the source of contamination in groundwater is affected by the complex interaction of climatic factors with the chemical and biological factors in the unsaturated zone.

Huyakorn et al. (1988) simulated the source variation of aldicarb for a field site on Long Island, New York. Their approach is based on the linkage of three models:

- (1) PRZM is a dynamic compartmental code, designed to simulate chemical movement in unsaturated soil systems within and below the root zone. It allows the user to perform dynamic simulations of potentially toxic chemicals, particularly pesticides, that are applied to the soil or plant foliage. Details of the PRZM code can be found in Carsel et al. (1984).
- (2) VADOFT (Huyakorn et al. 1988) is a 1-D finite element code which simulates transient infiltration and solute transport in the vadose zone underlying the root zone. The code formally solves the Richards equation for unsaturated flow and the convection-dispersion equation for single-species transport. VADOFT can be operated as a stand-alone program or linked with PRZM and SAFTMOD.
- (3) SAFTMOD (Huyakorn and Buckley 1988) is designed to perform areal, cross-sectional, and axisymmetric analysis of groundwater flow and contaminant transport in saturated porous media. SAFTMOD operates as a stand-alone code or in conjunction with (1) and (2) above.

The study simulated the geometry of a field site located on the south shore of the North Fork of Long Island near the town of Cutchogue in New York. A representative cross-section of the field site is depicted in figure 6. The top 30-cm layer was assumed to be representative of the root zone. The second layer is referred to as the vadose zone layer (195 cm). The bottom layer constitutes the saturated flow zone (7.2 m). A sequential simulation was performed using PRZM to assess the water balance and aldicarb transport through the root zone in response to natural rainfall (daily values). The vadose zone model, VADOFT, utilized the daily time series of water and solute fluxes from the root zone model as input and simulated the water and solute flux delivered to the water table. Specific details, including the parameters used, can be found in Huyakorn et al. (1988). Figures 7a-b. illustrate the simulated effect of dynamic rainfall patterns

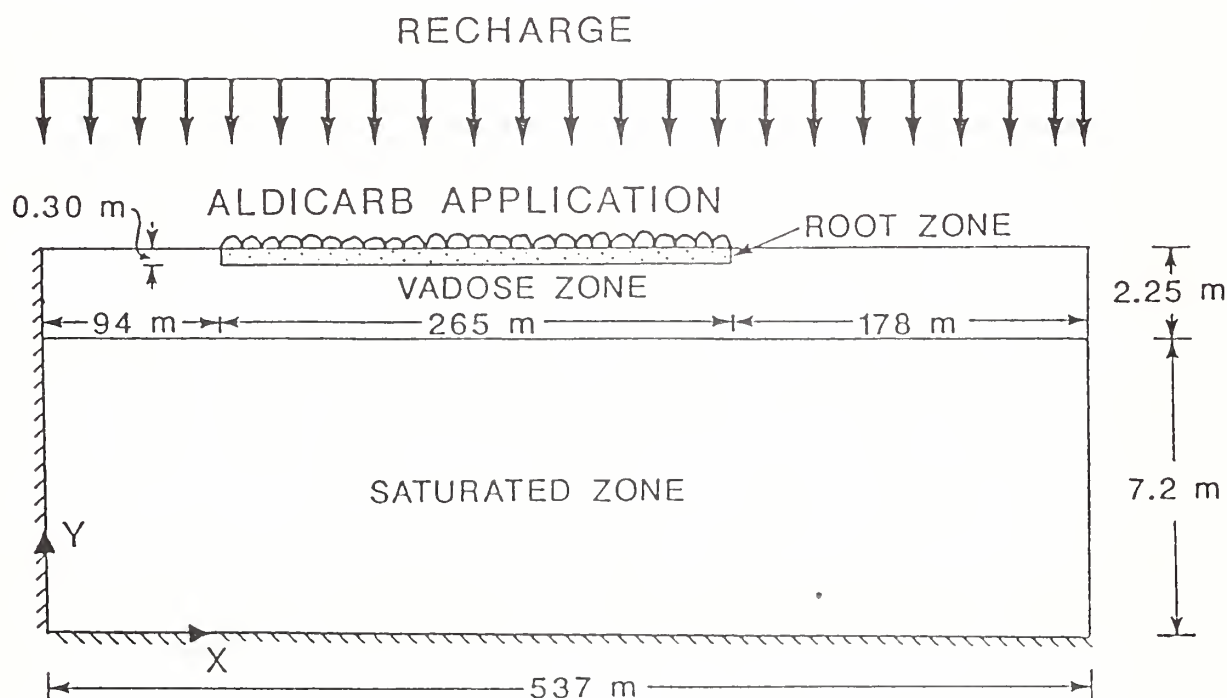


Figure 6.
A cross-section of the study site used for the simulation of aldicarb application and transport.

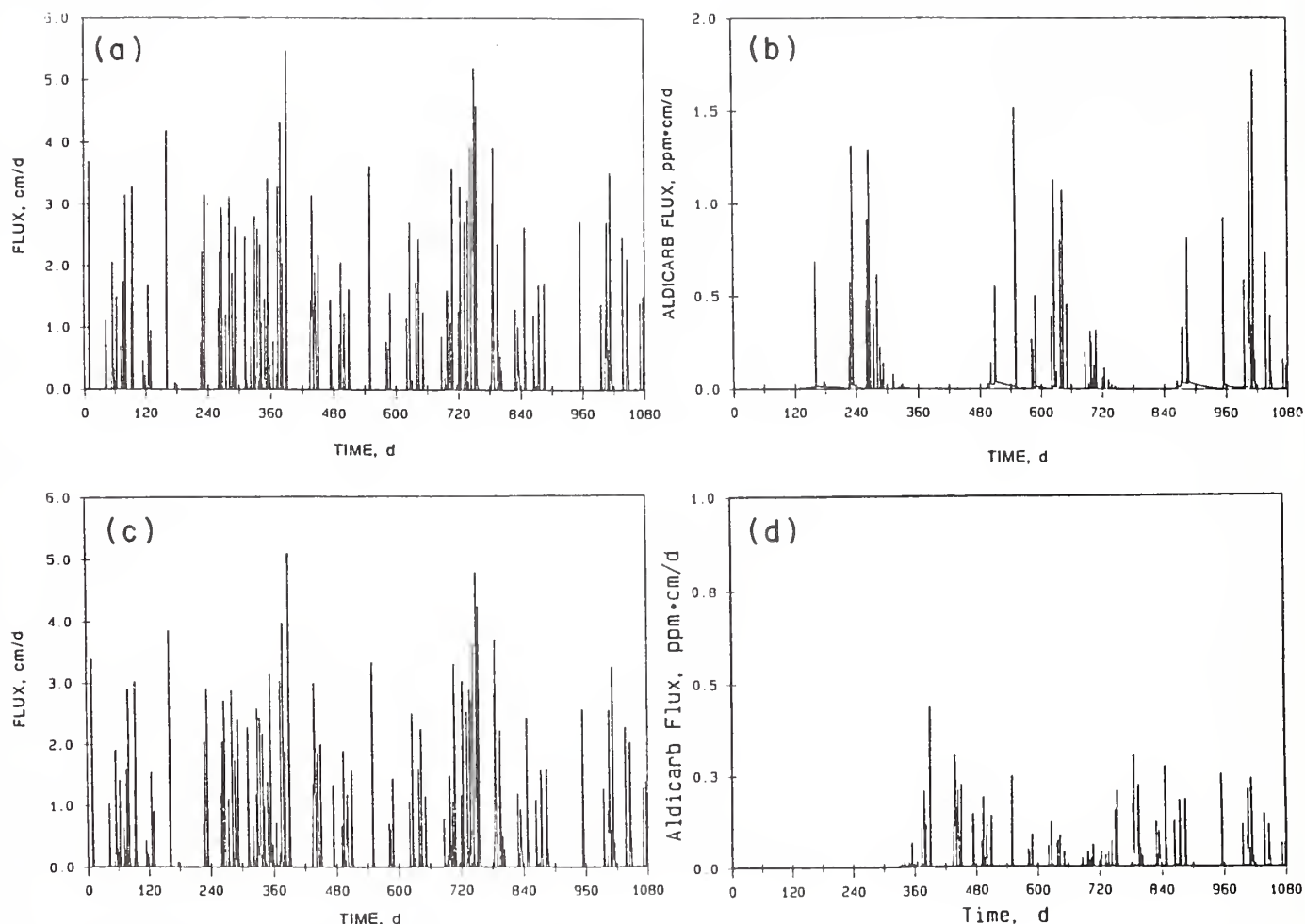


Figure 7.

(a) Simulated time series of water and (b) aldicarb flux at the bottom of the root zone for the period Jan. 1977 - Dec. 1979 (c) Simulated time series of water and (d) aldicarb flux at the bottom of the unsaturated zone and entering the water table.

on aldicarb transport and water flux through the root zone; figures 7c-d illustrate the solute flux from the unsaturated zone to the water table. The effect of dynamic forcing from precipitation and seasonal application of pesticide on source variability to the saturated zone is dramatically illustrated in this simulation. It is apparent that a substantial amount of aldicarb degradation and retardation can be expected in the unsaturated zone.

In almost every case of existing nonpoint-source contamination to groundwater, the spatial and temporal nature of the source is unknown. In this example we see how computer models can provide insight into the complex problem of source identification in the presence of complex climatic and geochemical interaction. Figure 8 depicts the average or mean monthly loading of aldicarb to the saturated zone, and the concentration contours which existed at the end of the simulation period.

SUMMARY AND CONCLUSIONS

The critical question for the problem of predicting nonpoint-source pollution at large scales is not so much the technical "Do we have the appropriate models?", but should address the conceptual framework "Do we understand the problem?". The fast pace of computational technology advancement during the last decade has set the stage for vigorous growth in theoretical and

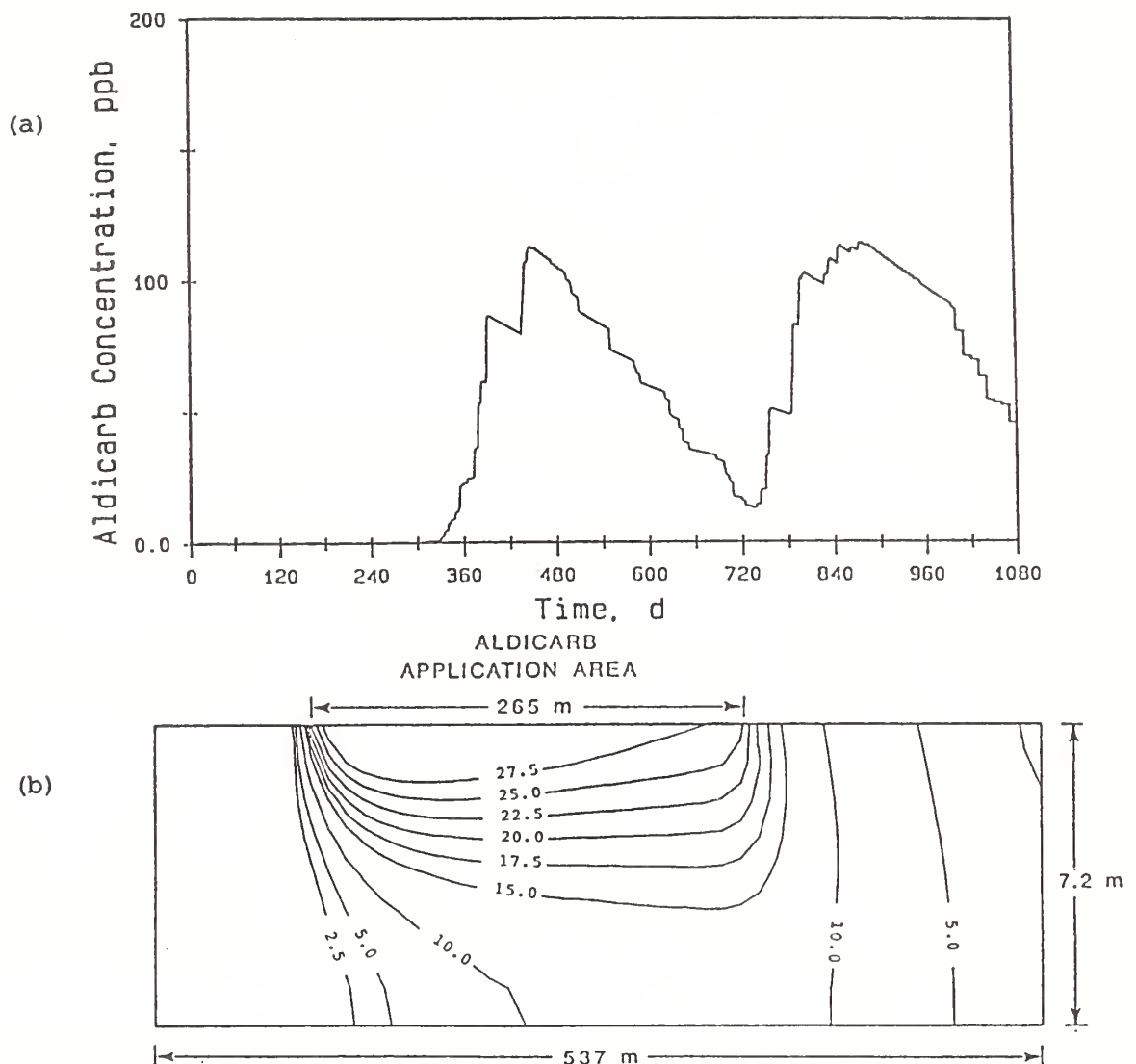


Figure 8.

(a) The time-averaged aldicarb concentration entering the aquifer.

(b) The concentration contours (ppb) at the end of the simulation

period ($t = 1080$ days). experimental aspects of environmental science and engineering. At present we are only beginning to make use of this resource, not only as a predictive tool, but to guide laboratory and field experiments and to search for practical simplification.

For the specific problem of predicting nonpoint-source contamination, it is reasonable to measure our progress in two areas:

Prediction/Experimentation

We need to consider the design and implementation of large-scale experiments, guided by current theoretical understanding but recognizing its limitations, if we are to better understand the problem of nonpoint-source contamination. It cannot be assumed that our experience and theories at the laboratory and field scales will provide predictions at the watershed or basin scales. Probabilistic, input/output, and multidimensional continuum models all play a role in the present day prediction capabilities of nonpoint-source pollution. However, it is not clear how previous

experiments and available data satisfy the needs of these computer codes (i.e., what is the minimum reliable data base necessary to insure reasonable predictions?). Sophisticated models of single- and multi-dimensional transport, coupled with mechanistic geochemistry can be used to gain insight into the relative importance of physical, chemical, and biological processes under idealized conditions. These models may also be used to test the sensitivity of solute prediction to various specific mechanisms of transport and chemical interaction, such as the influence of dispersive mixing when integrated results are sought.

Assessment/Controllability

By definition, diffuse sources of contamination are chronic hazards spread over large areas and contacting large volumes of soil and water, but usually at relatively low levels. On the other hand, point sources of contamination are localized, are often acute hazards requiring immediate attention, and for the most part only contact a small fraction of the water circulating in an aquifer.

From a public health point of view, it is not always appreciated that the physical differences between nonpoint- and point-source pollution require different approaches be taken for environmental management. For example, a localized point-source contaminant such as a waste plume emanating from a spill is often amenable to remediation, such as capture by pumping galleries and direct treatment. By contrast, an aquifer contaminated from a nonpoint source would require extraordinary effort and resources to apply active control because it might require the flushing of the entire aquifer. For most situations of nonpoint-source pollution, it seems likely that active control is limited to "source" control, while aquifer quality improvement must rely on natural flushing and dilution. One measure of flushing is residence time, which may vary from a few years for thin aquifers or high recharge up to centuries for thick aquifers or low recharge rates. Flushing may require several residence times for aquifer systems exhibiting reactive chemistry phenomena. Although the residence time evolves from the simple mixing cell theory, it has been shown that it can be related to parameters of physically-based models as well.

Model Limitations

It is apparent that much work needs to be done concerning spatial and temporal variability of the nonpoint-source term. However, it is unlikely that a precise identification of the source term will ever be possible. Numerical experiments offer one way to examine this impact on prediction; an example was presented here.

Geochemical reactions within the porous media account for the retention or mobilization of chemical species and are at least as important as physical transport processes. Concern over the long-term influence of nonpoint sources makes it imperative that we have a knowledge of specific reactions responsible for retention and mobilization. Accordingly, research on coupled mechanistic models of transport and geochemistry must continue if we expect to provide improved predictions. The computational complexity of direct and two-step approaches to coupling requires that more efficient approaches be examined. Future developments should also extend to kinetic based models and data bases as well. However, the nonpoint-source problem remains an interdisciplinary effort and fertile ground for research is found on the fringe between hydrological, geochemical, and soil science.

Finally, it is suggested that spatial integration may provide a practical tool for examining the coupled, dynamic effects of physical, chemical, and biological processes when used as an approximation to the more correctly formulated but idealized multidimensional numerical models.

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DISCUSSION OF PAPERS PRESENTED IN TECHNICAL SESSION 3, PART 1: GROUNDWATER MODELS FROM THE MODELER'S PERSPECTIVE

Charles Kinkaid¹, Presiding
Richard Peralta², Recorder

PAPERS DISCUSSED

Groundwater Quality Modeling for Agricultural Nonpoint Sources by I. Bogardi, J.J. Fried, E. Frind, W.E. Kelly and P.E. Rijtema

A Review of Groundwater Models for Assessment and Prediction of Nonpoint-Source Pollution by C.J. Duffy, C. Kinkaid and P. Huyakorn

SPECIFIC QUESTIONS AND COMMENTS

Question: (Audience) Your experiments assumed a constant source of contaminant. Most non-point-source (NPS) problems result from sources that vary with time. Is your experimentation applicable to such problems?

Response: (C. Duffy, Department of Agronomy, Cornell University, Ithaca, New York) Yes, exponential decay functions are applicable for both situations.

Question: (Audience) Biochemical reaction rates are nonlinear. How can one use linear equations in such models?

Response: (C. Duffy) We are trying to linearize the physical system -- a system which we understand very well. We are expressing the biochemical processes nonlinearly.

Response: (C. Kinkaid, Battelle Pacific NW Labs, Richland, Washington) Computational expense makes us use linear equations to the extent possible.

Comment: (Audience) The systems are too complex to be represented linearly.

Response: (C. Duffy) We are searching to simplify linear assumptions so that we can more feasibly run some of our simulations.

Response: (W. Kelly, University of Nebraska, Lincoln, Nebraska) Before one can say what simplification is acceptable, one must agree on the scale of the problem. Whether one is guarding one well or a large area makes a difference. Dispersion may or may not be important depending on the scale of the problem.

Response: (C. Kinkaid) It is very important to use simple models at this stage in geochemical modeling development.

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Comment: (Audience) Ignoring dispersion is going to be bad if one had diffuse as well as point sources.

Response: (C. Duffy or C. Kinkaid) We agree, but our work deals mainly with the point of outflow.

Comment: (Audience) Other similar experiments using known input and output functions gave linear results in the lab, but proved unacceptable for field use.

Response: (C. Duffy) It is very difficult to get appropriate probability distribution functions of the input and output signals.

Comment: (W. Kelly) One needs to realize how difficult it is to get data in the field. We must be realistic in terms of how much data we can expect to have and develop models appropriately. Decision-makers get stubborn when modelers say that they need more monitoring wells.

Response: (C. Duffy) Simple theory gives one simple rules to use to collect data. These provide rules of thumb.

Comment: (Audience) Time scales are very important.

Response: (C. Duffy) Simple models give one a sense for the residence time in the physical system.

Question: (Audience) What biodata exist in aquifers? Aquifers are not as dead as previously thought.

Response: (W. Kelly) In some cases in Nebraska denitrification is occurring. John Wilson at the EPA Ada, Oklahoma Lab shows that biochemical reactions are occurring. It is very necessary to have interdisciplinary efforts. Some Superfund technologies may be applicable.

Comment: (Audience) Microbial degradation does occur in groundwater. Degradation occurs even in the absence of microbes.

Question: (Audience) Is there much work underway to relate vadose zone modeling and groundwater modeling to better determine outflow to estuaries and streams?

Response: (C. Duffy) Such work is well underway. Important issues are comparing the rates of transport versus rates of degradation to determine residence times.

Comment: (C. Kinkaid) We need to measure outflow and calibrate that as well as heads. We need to monitor the quality of outflow.

Comment: (W. Kelly) It is fairly easy to measure and monitor outflows -- especially around sewage treatment areas.

Question: (Audience) Simple models are desired by bureaucrats. What happens when simple models do not give the expected answers?

Response: (C. Duffy) Our simple steady- and unsteady-state models give reasonable answers.

Comment: (C. Kinkaid) We must not stop at prediction. We must get to the point of actually comparing prediction with what happens in the field.

GROUNDWATER-QUALITY MODELS FOR PLANNING, MANAGEMENT AND REGULATION

Paul K.M. van der Heijde¹ and Thomas A. Prickett²

ABSTRACT

In the development of groundwater protection and rehabilitation strategies, mathematical models play an important role. This paper discusses the role of models in solving groundwater quality problems and explores issues related to the use of such models in planning, management, and regulation, with a focus on generic and site-specific nonpoint pollution of saturated groundwater systems. The applicability of various kinds of models to nonpoint pollution problems is discussed and an overview presented of pertinent, available models.

INTRODUCTION

In the last few decades, contamination of groundwater resources through the introduction of organic and inorganic chemicals, radionuclides, and microorganisms from domestic, industrial, and agricultural activities has become an increasingly significant environmental problem (EPA 1977, Jackson 1980, Pye et al. 1983, NRC 1984). Groundwater pollution may result from direct introduction of chemicals to the groundwater system or from other components of the water cycle (e.g., acid precipitation), and indirectly (often inadvertently) from induced alterations in water quality through modification of external or related system conditions (e.g., salt water intrusion and soil salinization resulting from irrigation).

A major source of groundwater pollution is the intentional or accidental introduction of solid and liquid wastes into near-surface soil or the deeper subsurface. Other major causes of groundwater pollution are the widespread use of such agricultural chemicals as pesticides, and fertilizers, and the production of manure, especially in feedlots. Irrigation return flow can contribute significantly to local and regional groundwater quality problems.

Sources of groundwater pollution can be distinguished in terms of their spatial, chemical, and physical characteristics, and their temporal behavior. The spatial definition of the source includes its location within or above the groundwater system, and its spatial extent. Often, pollution sources are divided on the basis of their relative spatial extent into point and nonpoint sources. Such a distinction is highly influenced by the scale on which the analysis takes place.

To understand the consequences of introducing pollutants in the subsurface and to evaluate protection and remediation scenarios, data analysis with mathematical models has become an important methodology in support of groundwater management resources.

In general terms, a model is a non-unique, simplified description of a part of the real world. A quantitative model of a specific groundwater system consists of mathematical descriptions of the relationships between the various components of the system, the active processes, and the internal and external stresses, combined with site-specific and process-specific data. In practice,

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the generic mathematical framework, coded in a programming language, is separated from the data and constitutes a generic groundwater model, sometimes referred to as a mathematical or computer model. The most complex of these computer models use numerical solution techniques to allow simulation of various combinations of coupled hydrologic, hydraulic, geochemical, and biochemical processes active in the heterogeneous near-surface and deep underground.

The rapid growth in the use of groundwater models has led to unforeseen problems in project management. Some projects in which these sophisticated tools have been used have even led to adversary legal proceedings in which the model application or even the model's theoretical framework and coding have been contested. Issues of concern include code model validation, code selection and prediction accuracy, project review and procurement, data requirements, information exchange, program maintenance, and training. Among other considerations, quality assurance and quality control (QA/QC) in model development, selection, and application and relying on well-trained professionals provide effective solutions to improving the usefulness of model predictions in terms of reliability and accuracy (van der Heijde and Park 1986, van der Heijde et al. 1988).

ROLE OF MODELING IN PROTECTING GROUNDWATER FROM NONPOINT-SOURCE POLLUTION

In the 1960's, as the rapid development of computer technology made it possible to efficiently simulate groundwater systems using software instead of physical scale models or electric analogs, modeling became an increasingly popular tool in groundwater management (Prickett 1975). From the beginning, the U.S. Geological Survey (USGS) has contributed significantly to groundwater modeling. The USGS established an analog model laboratory in Phoenix, Arizona in 1960 and more than 100 analog models were constructed during the next 15 years. In the late 1960's the USGS was the first to develop digital models to replace analog models (Pinder and Bredehoeft 1968). Since then, the USGS has developed a comprehensive suite of simulation and parameter estimation models, many of which are widely used worldwide. Numerous reports have documented USGS computer codes for the simulation of groundwater flow and for solute transport and heat transport in groundwater. An overview of the early USGS contributions to groundwater modeling was presented by Appel and Bredehoeft (1976). Recently, Appel and Reilly (1988) compiled a listing of all pertinent USGS models.

Because pumping is the major means of withdrawing groundwater, management is concerned with determining location, spacing, and sizing of wells or well fields, and the rates and time patterns of pumpage. Pumping may reduce the natural discharge of groundwater to streams and thus reduce base flow; or, if the volume pumped is large enough to lower water levels significantly, further exploitation of the resource may lead to land subsidence. Modeling assists in addressing complex questions such as the optimum design of well fields, quantitative studies of regional groundwater resources, and prediction of water level declines resulting from pumping withdrawals. The first computerized groundwater models were designed to evaluate the development of well fields in local and regional aquifer systems, while limiting the environmental impact of such development. This was soon followed by applications to construction site drainage, agricultural drainage, and irrigation (Walker 1978).

In the last decade, groundwater contamination by organic and inorganic chemicals, radionuclides, and microorganisms from domestic, industrial, and agricultural activities has become an increasingly significant environmental problem. As a result, groundwater management is concerned not only with the optimal utilization of groundwater resources, but with their protection for future utilization.

One of the challenges in protecting groundwater resources comes from the increasing detection of diffuse or nonpoint sources of contamination. This kind of pollution is caused by the widespread introduction of polluting chemicals to the subsurface (e.g., from the use of agricultural chemicals and from pollutants in precipitation), or results from the cumulative effect of a large number of closely spaced point sources (e.g., septic tanks, spills and waste disposal at industrial sites, and animal feedlots). Soil and groundwater transport models may provide a viable, if not the only, method to predict contaminant transport for this kind of problem. Some of the principal areas where mathematical models can assist in the management of groundwater protection programs are (van der Heijde and Park 1986):

- (1) assessing fate of chemicals in a variety of hydrogeologic environments and climatic conditions, e.g., leaching of agricultural chemicals to groundwater,
- (2) development and screening of regulations and policies,
- (3) delineating vulnerable areas and protection zones,
- (4) assessing effects of management practices in terms of exposure, hazard, damage, and health risks (e.g., agricultural impacts [Balek 1982], crop rotation, and chemical application rates and timing [Leonard and Knisel 1986]),
- (5) development of guidance documents, as for zoning, construction of potential sources of pollution, use of chemicals, and permit issuance and petitioning,
- (6) design and evaluation of monitoring and data collection strategies, and
- (7) screening of corrective action alternatives for existing contamination and design of selected remediation methods.

TYPES OF GROUNDWATER MODELS

Groundwater models can be divided into various categories, depending on model purpose and design. Apart from spatial resolution (one, two, or three dimensions), and temporal definition (steady-state flow or transport versus time-dependent behavior), models are distinguished by the processes they are designed to simulate (van der Heijde et al. 1985).

Process-Oriented Model Classification

Existing groundwater models, including those suitable for analyzing nonpoint pollution problems, fall into four broad categories:

- (1) flow models describing hydraulic behavior of single or multiple fluids or fluid phases in porous or fractured rock,
- (2) mass-balance models,
- (3) contaminant transport and fate models, and
- (4) hydrochemical models.

Flow models provide information on the potential movement of contaminants, due to the water-transmitting function of the subsurface. They simulate the movement of one or more fluids in porous or fractured rock. One such fluid is water; the others, if present, can be air (in soil) or immiscible nonaqueous-phase liquids (NAPL's) such as certain hydrocarbons. A special case of multifluid flow occurs when layers of water of distinct density are separated by a relatively small transition zone, a situation often encountered when sea-water intrusion occurs. Flow models are used to calculate changes in the distribution of hydraulic head or fluid pressure, drawdowns, rate and direction of flow (e.g., determination of streamlines, particle pathways, velocities, and fluxes), travel times, and the position of interfaces between immiscible fluids (van der Heijde et al. 1988).

Various physical, geochemical, or microbial processes control the movement of groundwater pollutants. Some processes pertain to the liquid phase, while others involve interactions between

the solid and liquid phase in the subsurface, between different fluid phases, or between the groundwater system and the atmosphere. Physical processes include advection and dispersion. The major geochemical processes are complexation, precipitation-dissolution, acid-base reactions, oxidation-reduction, and sorption. Sorption refers to two types of mechanisms, ion exchange or chemisorption, and physical adsorption and desorption of molecular species on colloid-size material. Biochemical processes that may occur in the subsurface include aerobic and anaerobic transformation of organic and inorganic compounds, often referred to as microbial degradation or decay (Jackson 1980).

Advection is the primary mechanism for migration of polluted water in the subsurface. Hydrodynamic dispersion (comprising mechanical dispersion and molecular diffusion; Bear 1972, 1979), often considered to be the cause of lateral spreading of the pollution, causes the front of a pollution zone to move forward at a rate higher than that of the bulk of the pollutants. Field-scale dispersion depends on distribution of the pore velocities and the characteristics of the rock reflected in the dispersivity distribution. Macroscopic or field-scale dispersion has been observed to be scale dependent, reflecting the variability of the pore velocities and the dependency of dispersivity on the heterogeneity of the rocks.

Geochemical processes might result in both reductions and increases of the concentration of pollutants. Some chemical processes remove one type of pollutant while creating or mobilizing another. Other processes occur as temporary phenomena, dependent on the physical and chemical state of the system. If the physical or chemical environment changes, e.g., from changes in temperature, pH, concentrations, or from the introduction of other chemicals, the initial effects of these processes may be reversed. Typical examples are adsorption-desorption and precipitation-dissolution. Also, when ion exchange occurs, the released ions themselves may be of a polluting nature (Konikow and Grove 1984).

Biodegradation in groundwater refers to chemical changes in solute or substrata due to microbial activity (Molz et al. 1986). Reactions can occur in the presence of oxygen (aerobic) or in its absence (anaerobic). The degradation products can also be major pollutants.

As advection and dispersion determine the zone and time available for chemical and microbial reactions to occur, the chemical and microbial processes, in turn, may affect the rate of other processes, as when adsorption retards the movement of a pollutant so that radioactive or microbial decay becomes more effective.

For some volatile chemicals, especially certain immiscible organics (e.g., aliphatic chlorohydrocarbons Schville 1984) and certain pesticides (e.g., Lindane), transport across the water-air interface at or above the water table may remove a significant part of the pollutants from the groundwater (Jury 1986).

Mass balance models provide information on the mass balance components and averaged concentrations of water soluble chemicals, based on the principle of conservation of mass.

Solute transport models provide concentration distributions for polluting chemicals subject to subsurface transport, and to chemical and microbiological transformation and degradation. A solute transport model uses velocities generated by a flow model or from (piezometric) head data by an internal subroutine to simulate advective displacement of a water-soluble chemical compound, sometimes allowing for additional spreading through dispersion and for transformations by chemical and microbial reactions. The transformations considered by so-called nonconservative models are primarily adsorption, radioactive decay, and biochemical transformations and decay.

The inclusion of geochemistry in solute transport models is often based on the assumption that the reaction rates are limited and thus depend on the residence time for the contaminant, or that the reactions proceed instantaneously to equilibrium. Recently, some researchers have become interested in a kinetic approach which incorporates chemical reactions in transport models, as some geochemical processes do not reach equilibrium during subsurface transport, especially in the unsaturated zone. This inclusion of geochemistry has focused on single reactions such as ion exchange or sorption for a small number of reacting solutes (Rubin and James 1973, Valocchi et al. 1981, Charbeneau 1981). Because multicomponent solutions are involved in most contamination cases, there is a need for a type of model that incorporates the significant chemical interactions and processes that influence the transport and fate of the contaminating chemicals (Cederberg et al. 1985). This is especially important in simulating fate of mixed pollutants.

Hydrochemical models represent the first type, as they consist solely of a mathematical description of equilibrium kinetics or reactions. These models, which are general in nature and are used for both groundwater and surface water, simulate chemical processes that regulate the concentration of dissolved constituents. They can be used to identify the effects of temperature, speciation, sorption, and solubility on the concentrations of dissolved constituents (Jenne 1981, Rice 1986).

As groundwater is part of a larger physical system, the hydrologic cycle, many models address in some way the interaction between groundwater and the other components of the hydrologic cycle. Some of these models describe only the interactions, sometimes as a process, sometimes as a dynamic stress or boundary condition. Increasingly, models are developed that simulate the processes in each subsystem in detail, in addition to the interrelationships (e.g., Morel-Seytoux and Restrepo 1985). Two types of models fit this latter category: watershed models and stream-aquifer models (sometimes called conjunctive-use models).

Watershed models customarily have been applied to surface water management of surface runoff, stream runoff, and reservoir storage. When water quality is included, these models allow for regional assessment of surface and subsurface effects of nonpoint pollution sources. Traditionally, however, these models did not treat groundwater in much detail, partly because of the wide range of temporal scales involved in adequately simulating the individual subsystems. The subsurface components in these models were limited to infiltration, water balances and solute mass balances, and to a lumped, transfer-function approach to determine groundwater flow and pollutant transport rates (e.g., El-Kadi 1983, 1986).

With the growing interest during the 1970's in the conjunctive use and coordinated management of surface and subsurface water resources by responsible authorities, a new class of models was developed: the stream-aquifer models, where the flow in both the surface water network and the aquifers present could be studied in detail. Increasingly, the coupled, deterministic submodels for determining stream stage and groundwater levels are now being linked with solute transport models. Recent interest in such multisystem modeling has grown, motivated largely by the need to simulate nonpoint pollutant transport (such as caused by the widespread use of agricultural chemicals) and by the need to study the contribution of local soil and groundwater pollution to the quality of surface water bodies. To model this type of problem, detailed (sometimes highly) descriptions of transport and fate processes for some of the subsystems are added to the multisystem flow models (e.g., Leonard and Knisel 1986).

An overview of watershed models having a significant watershed component is given in El-Kadi (1986). An overview of management models for conjunctive use is presented in van der Heijde et al. (1985).

Models designed for groundwater quality evaluation are used increasingly for analysis of health risks and environmental effects of potential or existing pollution. In this context, the model provides information regarding subsurface pathways and groundwater concentrations of pollutants

(e.g., see Mulkey et al. [1986] regarding pesticides, Whelan and Brown [1988] for RCRA applications, and Murphy [1982] on risk assessment modeling for hazardous waste sites). Some groundwater models are part of a multimedia exposure and risk analysis package (Cohen 1986).

Model Classification Based on Mathematical Methods

In modeling the transport of dissolved chemicals, the principle of mass conservation should be applied to each of the chemical constituents of interest. The resulting equations include physical and chemical interactions, as between the dissolved constituents and the solid subsurface matrix, and among the various solutes themselves (Reilly et al. 1987, Konikow and Grove 1984). To complete the mathematical formulation of a solute transport problem, equations are added describing groundwater flow and chemical interactions, as between the dissolved constituents and the solid subsurface matrix, and among the various solutes themselves. In some cases, equations of state are added to describe the influence of temperature variations and the changing concentrations on the fluid flow through the effect of these variations on density and viscosity.

Under certain conditions such as low concentrations of contaminants and negligible difference in specific weight between contaminant and the resident water, changes in concentrations do not affect the flow pattern (homogeneous fluid). In such cases a mass transport model can be considered as containing two submodels, a flow submodel and a quality submodel. The flow model computes the piezometric heads. The quality submodel then uses the head data to generate velocities for advective displacement of the contaminant, allowing for additional spreading through dispersion and for transformations by chemical and microbial reactions. The final result is the computation of concentrations and solute mass balances.

In cases of high contaminant concentrations in waste water or saline water, changes in concentrations affect the flow patterns through changes in density and viscosity, which in turn affect the movement and spreading of the contaminant and hence the concentrations. To solve such problems through modeling, simultaneous solution of flow and solute transport equations or iterative solution between the flow and quality submodels is required (Voss 1984, Kipp 1987).

In terms of spatial orientation, (sub-)models may be capable of simulating systems in one, two, or three dimensions. Temporally, they may handle either transient or steady-state simulations or both. Another distinction in the way models handle parameters spatially is whether the parameter distribution is lumped or distributed.

Lumped-parameter models assume that a system may be defined with a single (usually mean or "characteristic") value for the primary system variables. The system's input-response function does not necessarily reflect physical laws. Lumped parameter models mostly fit in one of two categories: (1) mass balance models, e.g., water balance or water budget models; and (2) system analytical or "black box" models, based on an empirical response function (Domenico 1972).

For both type of models, different levels of aggregation may be employed, from detailed multicompartment or multicell models to simple, single-cell models.

Most mathematical models used in groundwater management are distributed-parameter models, with deterministic and/or stochastic components. Increasingly, however, for assessment of uncertainties in complex systems (e.g., as in multimedia risk assessments or where the various components of the studied system require simulation with different spatial or temporal scales) lumped parameter models prove useful. The mathematical formulation of lumped parameter models often consists of a simple algebraic equation, easily embedded in other mathematical formulations, as for optimization.

In distributed-parameter models, the system variables often reflect detailed understanding of the physical relationships in the system and may be described with a spatial distribution. Here, system responses may be determined at various locations. Their mathematical framework consists of single or systems of partial differential equations called field equations, accompanied by initial and boundary conditions and solution procedures (Bear 1979). According to the solution method adopted, a distinction can be made between analytical models, semi-analytical models, and numerical models.

Analytical models contain a closed-form solution of the field equations, continuous in space and time. An important attribute of analytical solutions is the implicit conservation of mass (continuity principle). As analytical solutions generally are available only for relatively simple mathematical problems, using them to solve groundwater problems requires extensive simplifying assumptions regarding the nature of the groundwater system, its geometry, and external stresses (Walton 1984, van Genuchten and Alves 1982).

In semi-analytical models, complex analytical solutions are approximated by numerical techniques, resulting in a discrete solution in either time or space. Models based on a closed-form solution for either the space or time domain, and which contain additional numerical approximations for the other domain, are also considered semi-analytical models. This type of model includes those that provide streamline and traveltime information through numerical integration in space or time, of analytical expressions (e.g., Javandel et al. 1984).

In numerical models a discrete solution is obtained in both the space and time domains by using numerical methods to transform the field equations into a set of algebraic equations which are solved using direct or iterative matrix methods. If the equations are nonlinear, linearization often precedes the matrix solution (Remson et al. 1971, Huyakorn and Pinder 1983). Various numerical solution techniques are used in groundwater models. They include finite-difference methods, integral finite-difference methods, Galerkin and variational finite-element methods, collocation methods, boundary (integral) element methods, particle mass tracking methods (e.g., random walk), and the method of characteristics (Huyakorn and Pinder 1983, Uffink 1983, Kinzelbach 1986).

Until recently, most groundwater modeling studies were conducted using deterministic models based on precise descriptions of cause-and-effect or input-response relationships. Increasingly, however, models used in groundwater protection programs reflect the probabilistic or stochastic nature of a groundwater system to allow for spatial and temporal variability of relevant geologic, hydrologic, and chemical characteristics (El-Kadi 1987).

STATUS OF SOLUTE TRANSPORT AND FATE MODELS

Major criteria in selecting a model for a particular problem are (van der Heijde and Beljin 1988):

- (1) that the model be suitable for the intended use,
- (2) that the model be reliable, and
- (3) that the model can be applied efficiently.

To see if a model is suited for the intended use its characteristics must be well documented. The reliability of a model is determined by the level of quality assurance applied during its development, its verification and field validation, and its acceptance by users. A model's efficiency is determined by the availability of its code and documentation, and its usability, portability, modifiability, and economy with respect to human and computer resources required.

Appendix 1 presents a characterization of selected numerical solute transport models in the public domain. In selecting these codes, criteria discussed by van der Heijde and Beljin (1988) and van der Heijde et al. (1988) have been applied. For each model the type of rock and source characteristics, and boundary, fluid, and flow conditions to which it can be applied are given. The tables include a summary of the transport and fate processes that are included in models. In addition, the model's geometry and simulation capabilities are listed. Additional information regarding the availability of simulation models for flow and transport in unsaturated and saturated subsurface systems can be found in van der Heijde et al. (1988).

MODELING AREAL SOURCES OF GROUNDWATER POLLUTION

In modeling areal sources of groundwater pollution, the source must be described in terms of its spatial, chemical, and physical characteristics, and its temporal behavior. The spatial definition of the source includes location, depth, and areal extent, and together with the scale of modeling identifies the source as a point source, a line source, a distributed source of limited areal or three-dimensional extent, or as a nonpoint source of unlimited extent (van der Heijde 1986). The areal extent of the source in relation to the scale of modeling determines the spatial character of the source in the model. In some cases a nonpoint pollution source for a local scale model is considered a point pollution source for modeling at a regional scale (e.g., individual septic tanks, landfills, feedlots).

In the model, the source can be placed at the boundary or within the system for which the model is developed. In this respect, the choice of system boundaries is important: a source located in the unsaturated zone is an internal source for a model that includes this zone, but is also a boundary source for a model of the saturated zone alone. Not only are different types of models required (variably-saturated versus saturated-zone models), but the models need to describe the source in different mathematical ways, i.e., as an internal source or as a boundary condition, respectively. Also, the choice of the spatial model characteristics (e.g., two-dimensional versus three-dimensional) influences the way boundaries are simulated (fig. 1).

Another source characteristic important to the modeling process is its history or expected temporal behavior. The source can be continuous in time, either fluctuating or constant in strength (e.g., landfills, impoundments, feedlots), or in the form of a pulse or series of individual, nonoverlapping pulses (e.g., spills, leaching of agrochemicals during or after a storm).

In addressing the use of models in the protection of groundwater from nonpoint pollution sources, a distinction can be made between generic and site-specific modeling. If the problem studied is site-specific, e.g., pertinent to a particular location (or site), the data required will result from a detailed characterization of that site. Where the results of environmental analysis must be applied to many sites (e.g., in analyzing the impacts of new environmental regulations), where data availability is limited, or where other constraints are present (e.g., limited computer resources, project time, and expert staff), site-specific modeling is inappropriate or often not feasible. As a result, two major approaches exist to this kind of modeling. In one approach, decisions are made by applying models to generic formulations of management issues and to generic definitions of the groundwater systems, often based on average or worst-case hydrogeologic conditions coupled with sensitivity analysis. The models used for this type of analysis can be rather complex and may include numerical models. An example is the comprehensive study of the nitrogen cycle in the subsurface in areas of heavy fertilizer use, extensive land treatment of wastewater, and a large number of animal feedlots (e.g., Frissel and van Veen 1981, Iskander 1981).

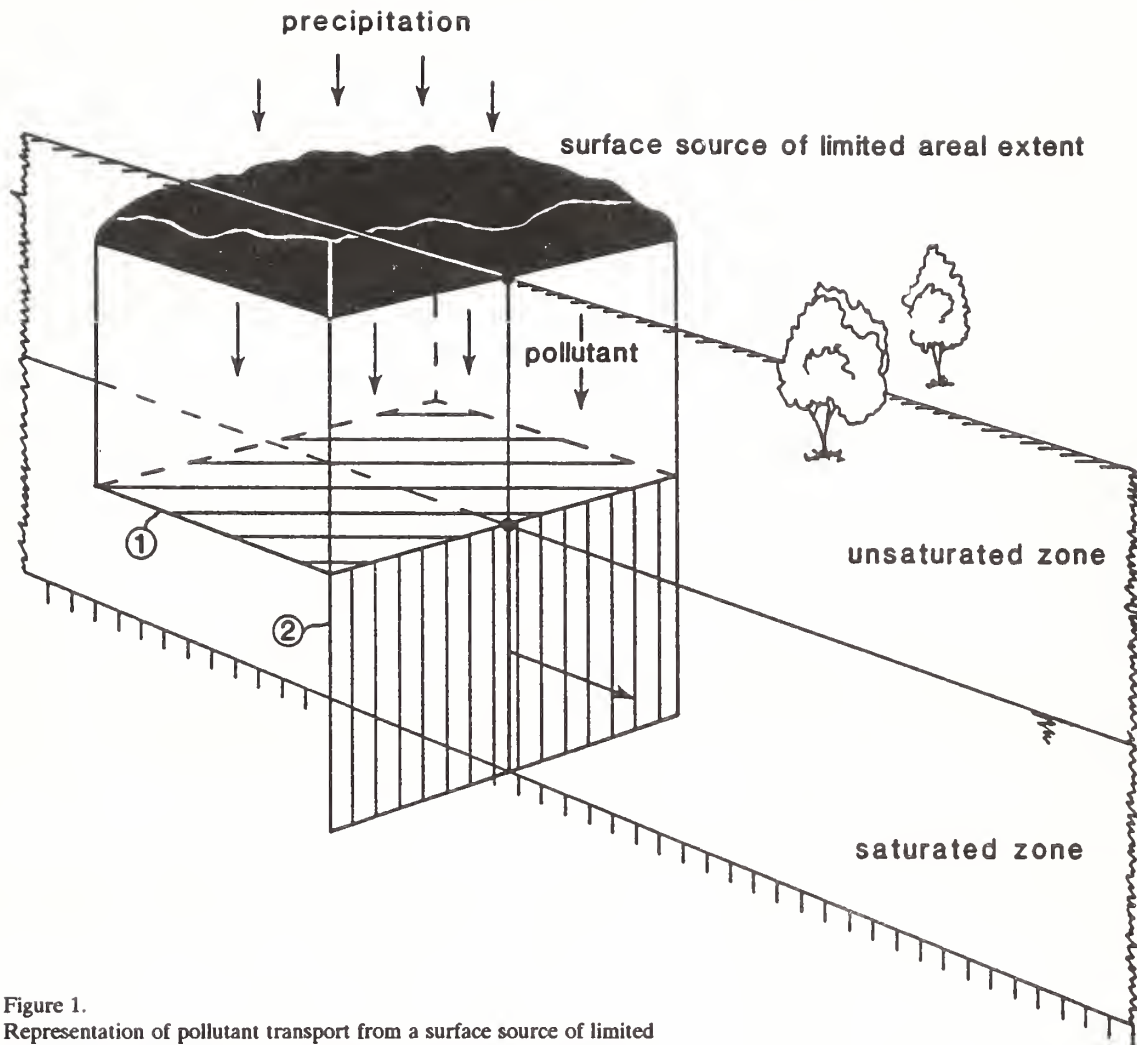


Figure 1.
Representation of pollutant transport from a surface source of limited areal extent in a saturated-zone model: (1) horizontal areal source underneath surface source at the top of an aquifer; (2) vertical source area at edge of projected surface source area in the aquifer.

In the second approach analytical models are applied, often in the form of stochastic analysis, to a large number of simple datasets representing a wide variety of field conditions (e.g., EPA 1986). The cost of such exercises would in most cases be prohibitive when using numerical models. However, the limitations imposed by analytical models on the simulation of a complex groundwater system require restraint in the use of computed results. Therefore, in choosing representative scenarios and model input, or in selecting statistics-based decision criteria, a so-called "conservative" approach is frequently taken.

Although most models used in groundwater studies are based on a spatially distributed definition of the parameters (either in a deterministic or stochastic framework), for analysis of nonpoint pollution lumped-parameter models have been applied successfully in studies of the effects of the unsaturated zone on the transport of contaminants from the surface to the groundwater table (Novotny 1986); to simulate the contribution of the subsurface to surface water pollution (e.g., Bendoricchio and Rinaldo 1986); and to determine the application period for chemicals on arable land based on groundwater protection considerations (Antal et al. 1987).

Another approach to modeling groundwater pollution from diffuse sources is described by Kaden (1987). To account for the variety of management needs and the complexity of groundwater systems, a model hierarchy is described, distinguishing between planning models, management models, and operational models. Planning models are based on a high level of abstraction (or simplification) of the groundwater system and are designed for the analysis of long-term policies applicable to regional or larger areas. Management models are applied to mid-term planning horizons and have a regional or even local application, as for the management of water quality affected by seasonal irrigation. Finally, operational models are for the analysis of short-term scenarios, e.g., to determine the need for and the duration of daily irrigation applications, using daily weather forecast information.

A distinction is sometimes made between research models, screening models, and management models. Here, screening models are comparable to Kaden's planning models; the management models include both Kaden's management and operational models; and a new group, research models, accounts for a large group of models developed to study the fundamentals of underlying subsurface processes and the numerical techniques to solve the resulting mathematical formulations. Research models often focus on specific processes or systems that have been highly simplified or even hypothetical. Consequently, these codes are not often applicable to field problems. Often, research models form the basis for development of management models (e.g., Davidson et al. 1978) or are used to validate the management models for the range of conditions and parameter values to which the model is applicable (e.g., Wheeler et al. 1987).

SCALES IN GROUNDWATER MODELING

A major aspect of the application of models is defining the spatial and temporal scales to be used in the model. Different scales might apply to various subsystems simulated by the model. The selection of scales depends on the objectives of management, the nature of the system(s) modeled, and the chosen numerical method, among other considerations.

In general, human-induced influences on groundwater systems affect local and intermediate scales, while large, regional-scale phenomena are of natural origin. Some human-induced changes are also on a regional scale, such as the amalgamated effect on water levels and return flow of groundwater withdrawal for irrigation; nonpoint pollution caused by use of fertilizers and pesticides in agriculture; acidification of groundwater as a result of acidic precipitation; and the changes in groundwater quality resulting from urbanization.

The essential scaling problem is how to distinguish between the variables that can and those that cannot be considered as constants or as being uniform across discrete intervals of pertinent dimension (space, time) (Beck 1985). Problem decomposition in space or time is often applied to obtain optimal resolution in relation to computational efficiency. An example of such spatial and temporal decomposition is found in the modeling of infiltration into the soil and subsequent percolation toward the saturated zone. A distinction has been made between spatial discretization and connectiveness in the presence of nonpoint sources for local (fig. 2) and for regional (figs. 3a and 3b) scales (van der Heijde 1988). Runoff from precipitation is split into a surface component (lumped horizontal segment) and infiltration (one-, two-, or three-dimensional, vertical).

The infiltrated water percolates to the groundwater where a two-dimensional horizontal or three-dimensional model is used. A different timestep is used for each of the submodels, from hourly for the surface runoff and daily for the percolation, to weekly or monthly for the flow in the saturated zone.

Note the difference in treatment of the vertical components in groundwater models. In the regional models (figs. 3) the flow in soils and between aquifers is mainly one-dimensional and

vertical, to reduce the computational load. Here, the flow between aquifers is generally represented by a single unit while the flow in soils might be vertically discretized. In local models (fig. 2), second-order effects may be important enough to justify the use of two-dimensional vertical or three-dimensional simulation in the soil zone.

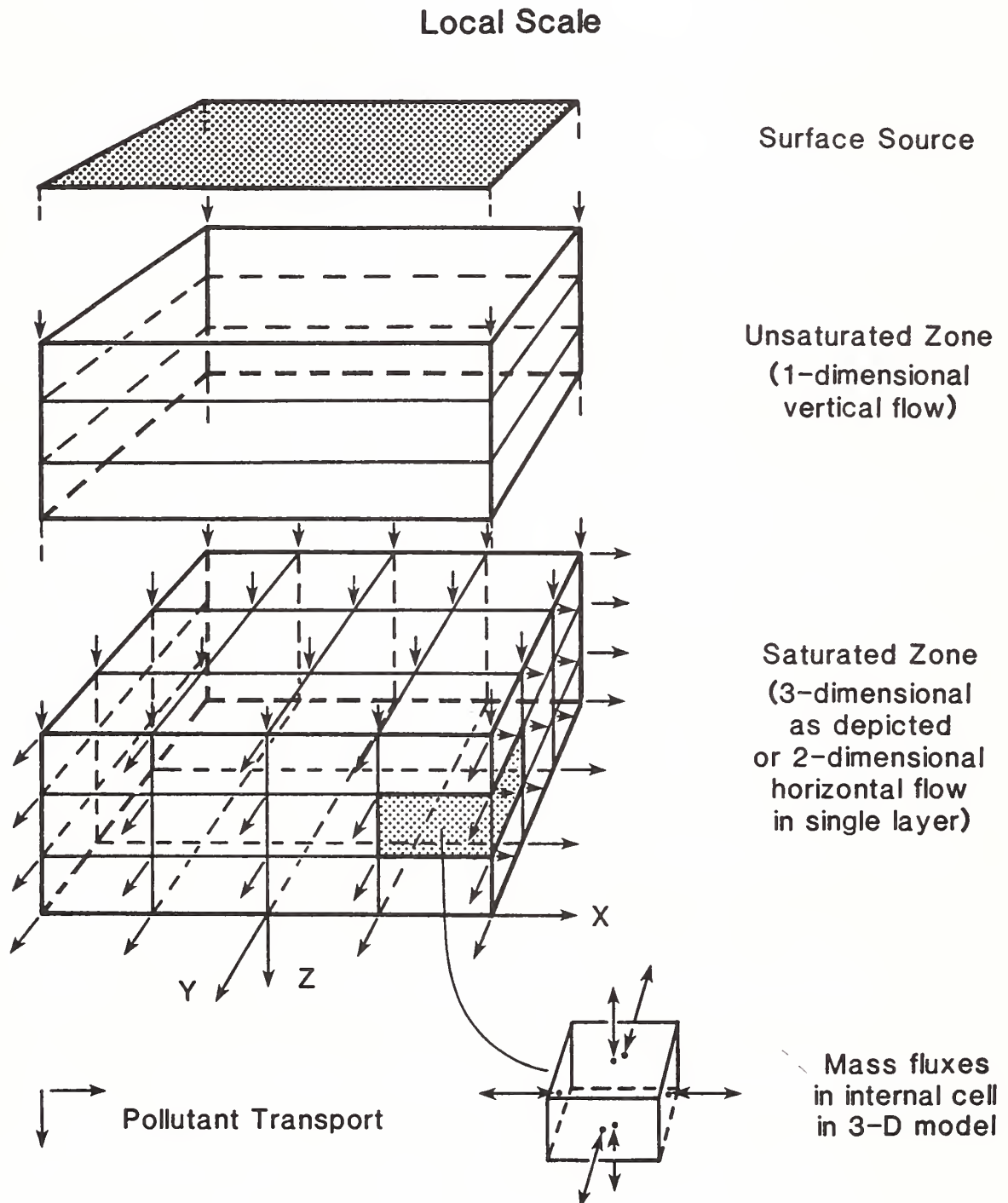


Figure 2.
Typical schemes used to represent a single-area surface source in simulating pollutant transport in the unsaturated and saturated zones, using local-scale groundwater models.

Regional Scale – Constant Discretization

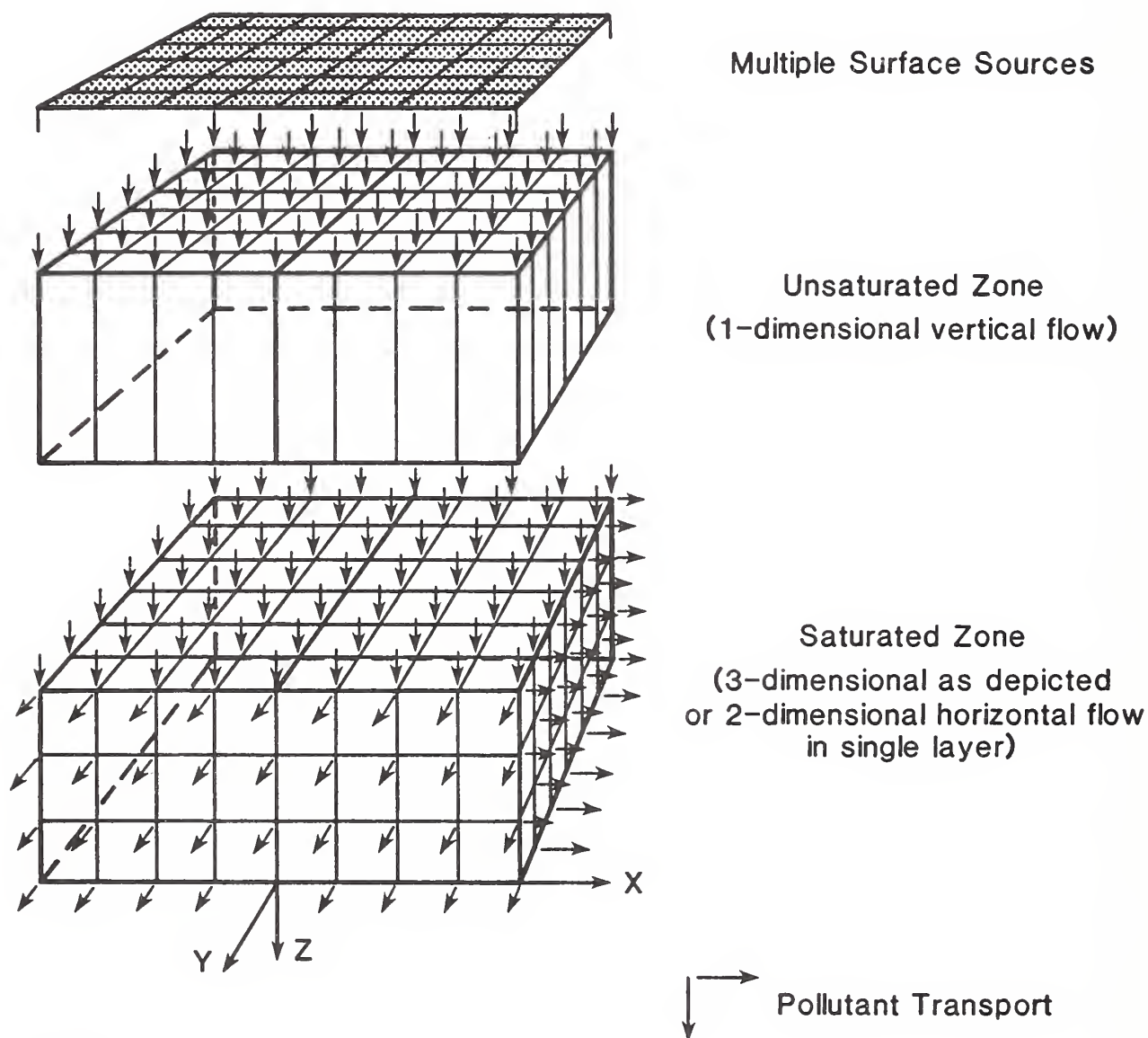


Figure 3a.
Typical schemes used to represent a multi-area surface source in
simulating pollutant transport in the unsaturated and saturated zones,
using regional-scale groundwater models; constant discretization.

ISSUES IN AND LIMITATIONS OF GROUNDWATER MODELING

Accurate modeling of groundwater pollution is limited by some fundamental problems. In the first place, not all processes involved are adequately described mathematically (Bear 1988). For the most complex mechanisms, available numerical techniques are not always adequate (Pinder 1988). Finally, in most cases, lack of quantity or quality of data restricts model utility (Bear 1988, Konikow 1988).

Improvements are required, concurrently, in several other major areas. Data acquisition methods and interpretive models are needed that can examine to an unprecedented degree the physical,

Regional Scale – Varying Discretization

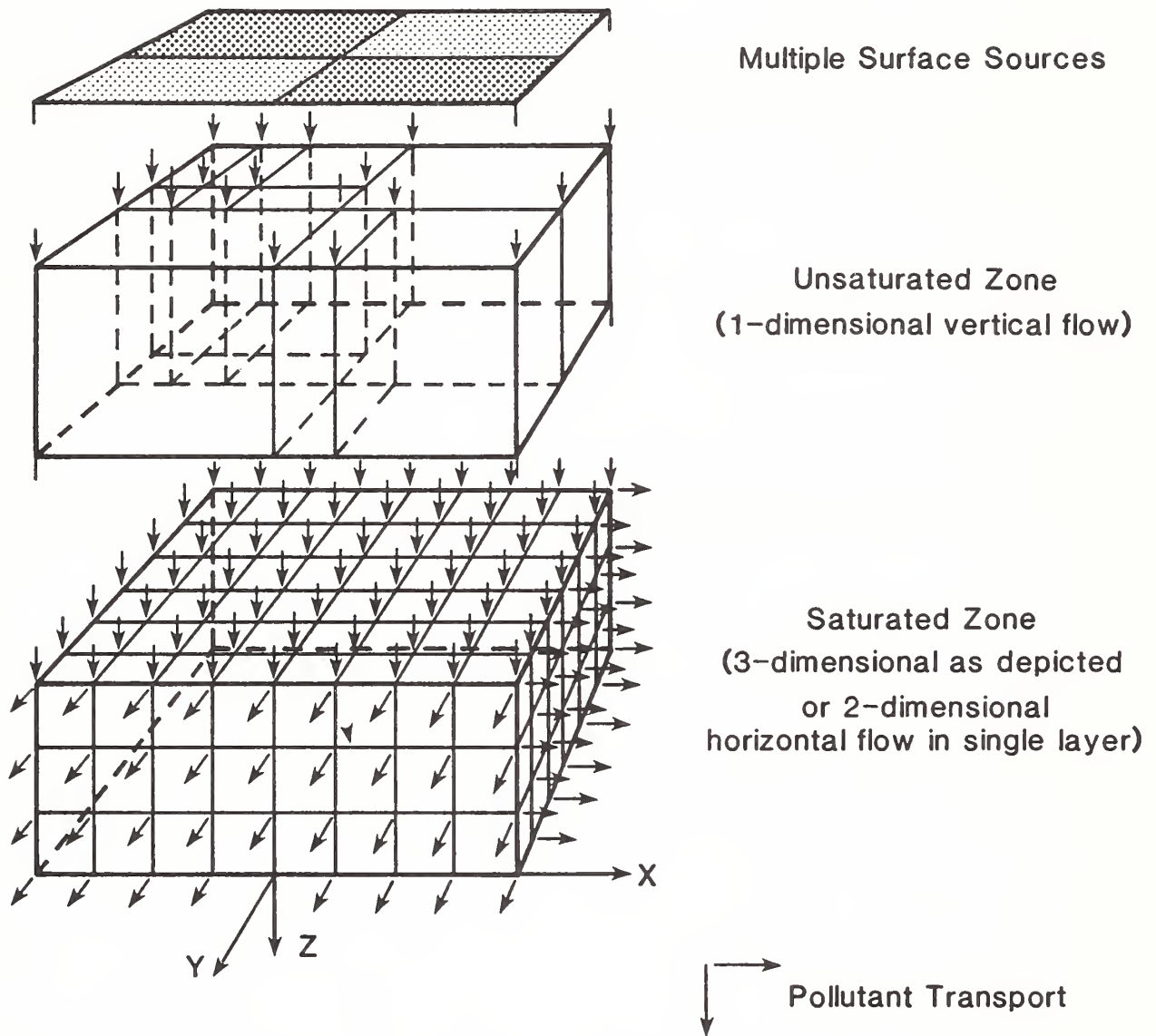


Figure 3b.
Typical schemes used to represent a multi-area surface source in simulating pollutant transport in the unsaturated and saturated zones, using regional-scale groundwater models; varying discretization.

chemical, and biological processes controlling the transport and fate of groundwater contaminants. Unfortunately, few of the constants and coefficients needed to incorporate chemical and biological processes into contaminant transport and fate evaluations are available.

The Role of Data

Modeling provides a framework to order and interpret data within the decision-making process. The effectiveness of any model depends on the accuracy of the utilized data. In many applications, the lack of data inflicts a severe constraint upon obtaining useful model results. Therefore, the

use of computer models in groundwater-resource development and protection will continue to be limited mainly by the time and costs incurred in collecting sufficient and accurate hydrologic and geologic data for proper description of groundwater systems and their functional characteristics. This does not mean, however, that some indication of the relative contribution of various processes to a groundwater system's total response cannot be estimated; much of the existing information can be used in a semi-quantitative manner (i.e., sensitivity analyses and "worst-case" scenarios).

A common misconception is that all field methods and tools necessary for obtaining data to run the models are available--if not in optimal form, at least in a useful form. In fact, however, direct measurements are unreliable or cannot be obtained for a number of parameters such as groundwater flow velocity and direction, rates of sorption and desorption (retardation) of organic chemicals, and the potential for biotransformation.

The use of newly developed theories to help solve field problems is often a frustrating exercise. Most theoretical advances call for some data not yet practically obtainable (e.g., chemical interaction coefficients and relative permeabilities of immiscible solvents and water). In addition, the incorporation of theoretical relationships into mathematical models typically is made possible by invoking certain assumptions and simplifications that alter the intended relationship. Therefore, theoretical advances in modeling groundwater problems must be accompanied by improvements in data collection and mathematical representation efforts.

Complex numerical models are particularly data-hungry. Incorporating new geochemical, hydrological, and biochemical processes often stretches existing data collection capabilities beyond a practical limit. Many cases require generic data obtained from laboratory batch experiments or controlled field experiments. Centralized management of such datasets and efficient dataset referral services are of great importance to the groundwater modeling community.

Management Concerns

Although models have become widely accepted, useful tools for drawing scientific conclusions and making technical decisions, models have not yet achieved great acceptance in the formulation of public policy. There are several reasons for the failure of policy makers to utilize models (OTA 1982, van der Heijde et al. 1985). Individuals at high levels of decision making (where policies are formulated) are often less familiar with models than the operation managers who use them for engineering decisions. Furthermore, policy decisions are increasingly contested in court. Evidence requirements in the litigation process are often difficult to meet, restricting management from incorporating modeling in their decision making. Opposing parties in a court of law frequently arrive at significantly different conclusions, sometimes based on results from the same model, thus contributing to management's reluctance to rely on models.

Management's lack of confidence in modeling probably reflects experience with unsuccessful model application. Failures have been attributed to (OTA 1982, van der Heijde et al. 1985, van der Heijde and Park 1986):

- (1) use of insufficient or incorrect data,
- (2) incorrect use of available data,
- (3) inadequate conceptualization of the physical system such as flow in fractured bedrock,
- (4) use of invalid boundary conditions,
- (5) selection of an inadequate computer code,
- (6) incorrect interpretation of the computational results, and
- (7) providing answers to imprecise or wrongly posed management problems.

Examples of these issues are contained in the findings of a study group for the EPA Office of Environmental Processes and Effects Research. The group examined issues related to that Agency's use of groundwater models and associated constraints (van der Heijde and Park 1986). According to the study group's report, the issues addressed can be divided into three major groups:

- (1) the computer model being used,
- (2) application (conceptualization, data selection, and simulation), and
- (3) use of computational results in decision making.

Issues of the first group included the assessment of the validity of computer codes. Prominent issues of the second group are criteria for selection of appropriate models for specific applications and review procedures for establishing model application adequacy and validity. The third group of issues relates only in part to modeling, as decision making is often based extensively on nontechnical considerations. A major limitation in addressing these issues is the scarcity of trained staff in all levels of management and technical services, both in government agencies and in private industry. To resolve many of the problems identified, the study group recommended that the Agency adopt rigorous, well-defined quality assurance procedures and establish extensive technology transfer and training programs.

The Role of Quality Assurance

The economic consequences of model predictions and the potential liabilities incurred by their use have brought quality guarantees and code credibility to the forefront as major issues in groundwater modeling. Hence, quality assurance (QA) needs to be defined and implemented for both model development and model application. There is a significant difference between these two: the first is designed to result in a generally reliable code, and the second to obtain reliable predictions for existing field conditions under prevailing management constraints. Both require stringent QA procedures. To further increase the applicability of the models, good documentation and user-friendliness of the computer coding involved should receive close attention.

Quality assurance is the procedural and operational framework put in place by the responsible organization, to assure technically and scientifically adequate execution of all tasks included in the project, and to assure that all project results (e.g., all modeling-based analyses) are verifiable and defensible (Taylor 1985). QA in groundwater modeling is crucial to both model development and model application and should be an integral part of project planning. The two major elements of quality assurance are quality control (QC) and quality assessment (van der Heijde 1987). Quality control refers to the procedures that ensure the quality of the final product. These procedures include the use of appropriate methodology, adequate validation, and proper usage of the selected methods and models.

To monitor the implementation of quality control procedures and to evaluate the quality of the studies, quality assessment is applied. It consists of two elements: auditing and technical review. Audits are administrative procedures designed to assess the degree of compliance with QA requirements, commensurate with the level of QA prescribed for the project. Compliance is measured in terms of traceability of records, accountability (approvals from responsible staff), and fulfillment of commitments described in the QA plan of a project. Technical review consists of independent evaluation of the technical and scientific basis of a project and the usefulness of its results. In groundwater modeling, this latter form of quality assessment is rather common (van der Heijde 1987).

Many modeling studies are performed without adequate QA arrangements in place; QA plans are often lacking and formal QA assessment is frequently postponed until the project reaches its final stage (see van der Heijde and Park 1986). This is especially true for studies where models are

applied to site-specific problems. In contrast, policies based on modeling assessments often affect large constituencies and thus are more carefully scrutinized before they are adopted. Increasingly, financial and criminal liability require modelers to implement rigorous QA procedures in all stages of a modeling project.

Frequently mentioned reasons for QA deficiencies are lack of specifications from management with respect to the level of analysis required for decision making; shortages of time, budget, and experienced staff; unfamiliarity with QA procedures; and reluctance to accept additional administrative duties (van der Heijde and Park 1986).

MODELING OUTLOOK

Several new developments are occurring in groundwater modeling. Groundwater flow models have evolved to a point where a wide range of flow characterizations is possible. The newer models may include options for various types of boundary conditions as well as the ability to handle a wide variety of hydrologic processes such as evapotranspiration, stream-aquifer exchanges, spatial and temporal variations in recharge, and the more complex characterization necessary for simulating unsaturated flow. Similarly, recently developed models for simulation of solute transport or new versions of earlier models often include increased flexibility in describing the solute source and simulating such transport and fate processes as radioactive decay or chemical transformation and effects of both equilibrium and kinetic adsorption. In some instances these transport models are coupled with existing geochemical models to provide a more complete analysis of the solute chemistry. Such a development has also been applied to the simulation of biodegradation, e.g., for the analysis of bioremediation schemes (Borden and Bedient 1986, Borden et al. 1986). Furthermore, important developments have occurred in the modeling of flow and transport in fractured rock systems. Here, both improved site characterization and stochastic description of fracture geometry, together with an improved capability to describe the interactions of chemicals between the active and passive fluid phases and the rock matrix, have enhanced the utility of model simulations in the study of real-world fractured rock systems. Multiphase flow models have become increasingly available, especially those designed for studying the movement of immiscible fluids such as NAPL's (van der Heijde et al. 1988). Also, new approaches have been developed for parameter identification and are increasingly used in practical applications (Yeh 1986). Finally, optimization-based management models have been applied to a growing variety of decision problems, especially in the area of groundwater protection (Wagner and Gorelick 1987).

Current and near-future research on geochemical, hydrological, and biophysical mechanisms, including large-, intermediate- (e.g., artificial aquifers), and field-scale experiments, will lead to further sophistication of mathematical tools for analysis of a variety of groundwater problems, considering the stochastic nature of many of the processes involved. The complexity of the resulting models will require a significant increase in computer resources, validation opportunities, and user expertise. Datasets generated in field-scale experiments will be particularly useful for retrospective model validation.

Recent modeling developments have raised many new areas of research. Fundamental research supporting groundwater modeling is necessary in such areas as:

- (1) spatial variability and transient behavior of process parameters (e.g., retardation, hydraulic conductivity),
- (2) desorption for nonhydrophobic chemicals,
- (3) multicomponent transport and chemical interaction,
- (4) improved numerical accuracy, stability, and efficiency,
- (5) efficient linkages between submodels of the hydrologic system, considering their different spatial and temporal scales, and
- (6) effects of aggregation of local-scale processes in regional models.

Parallel with and to a significant extent responsible for the rapid increase in groundwater modeling capabilities has been the technological advance in computer hardware and software. This is especially noticeable in the integrated approach to computer-based decision-support systems in groundwater management. In these hardware-software systems, data acquisition and control is combined with analytical, optimization, and presentation techniques, resulting in an efficient management tool. The recent introduction of artificial-intelligence-based expert system technology promises further advances in the utility and sophistication of decision-support technology.

Thus, many new opportunities and challenges in groundwater modeling will present themselves in the near future. The use of computer models in groundwater resource development will continue to be limited mainly by the costs of collecting sufficient and accurate hydrologic and geologic data for proper description of groundwater systems and their functional characteristics. Along with the growing complexity of groundwater models and methodologies, user expertise must expand through education and training.

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APPENDIX 1

Table 1A.

Features of major public domain numerical transport and fate models, from van der Heijde et al. 1988.

Model Characteristics	FEM- TRAN	FEM- WATER/ WASTE	PORFLO	GS2/ GS3	PRZM	SUMATRA SESOIL	-1	SUTRA
<u>Soil/Rock Characteristics</u>								
Confined aquifers	-	X	X	X	-	-	-	X
Aquitards	-	X	X	X	-	-	-	X
Watertable aquifers	X	X	-	X	-	-	-	X
Multiple aquifers	-	X	X	X	-	-	-	X
Heterogeneous	X	X	X	X	-	-	-	X
Anisotropic	X	X	X	X	-	-	-	X
Fractured	-	-	-	-	-	-	-	-
Single soil layer	X	X	-	X	X	X	X	X
Layered soils	X	X	-	X	X	-	X	X
Matrix deformation	-	-	X	-	-	-	-	-
<u>Fluid Conditions</u>								
Single fluid	X	X	X	X	X	X	X	X
Multiple fluids	-	-	-	-	-	-	-	-
Miscible	-	-	-	-	-	-	-	-
Immiscible	-	-	-	-	-	-	-	-
Freshwater	-	-	-	-	-	-	-	-
Salt water	-	-	-	-	-	-	-	-
NAPL ¹	-	-	-	-	-	-	-	-
Gas/air	-	-	-	-	-	-	-	-
Varying density	-	-	X	-	-	-	-	X
<u>Flow Conditions</u>								
Saturated	X	X	X	X	-	-	X	X
Unsaturated	X	X	X	X	X	X	X	X
Steady state	X	X	X	X	X	X	X	X
Transient	X	X	X	X	X	X	X	X
<u>Geometry</u>								
1-Dimensional								
-Horizontal								
(vertically averaged)	-	-	-	-	-	-	-	-
-Vertical								
(cross-sectional)	-	-	-	-	X	X	X	-
2-Dimensional								
-Horizontal	-	-	X	X	-	-	-	X
-Vertical	X	X	X	X	-	-	-	X
3-Dimensional	-	-	-	X	-	-	-	-

¹Non-Aqueous Phase Liquids

Table 1A (continued).

Model Characteristics	FEM- TRAN	FEM- WATER/ WASTE	PORFLO	GS2/ GS3	PRZM	SUMATRA SESOIL	-1	SUTRA
<u>Transport and Fate Processes</u>								
Advection	X	X	X	X	X	X	X	X
Dispersion	-	X	X	X	X	-	X	X
Matrix diffusion	-	-	-	-	-	-	-	-
Retardation	-	X	X	X	X	X	X	X
Non-lin. adsorption/ desorption	-	-	-	-	X	X	X	X
Ion exchange	-	-	-	-	X	-	X	-
Biotransformation/ degradation	-	-	-	-	X	X	X	-
First-order radioactive/ (bio-)chemical decay	X	X	X	X	-	-	X	X
Chemical reactions/ hydrolysis	-	-	-	-	-	X	-	-
Complexation	-	-	-	-	-	-	-	-
Volatilization	-	-	-	-	X	X	-	-
Heat/energy transport	-	-	X	-	-	-	-	X
<u>Boundary/Source Characteristics</u>								
Point source	X	X	X	X	X	X	X	X
Line source	X	X	X	X	-	-	-	X
Limited area or volume source	-	-	X	X	-	-	-	X
Areally distributed source	-	-	X	X	-	-	-	X
Specified source rate	X	X	X	X	X	X	X	X
Specified concentrations (or concentration function)	X	X	X	X	X	X	X	X
<u>Capabilities</u>								
Contaminant mass/rate of release to groundwater from unsaturated zone	X	X	-	X	X	X	X	X
Contaminant plume extent	-	-	X	X	-	-	-	X
Contaminant concentrations								
-as a function of distance from source	-	X	X	X	-	-	-	X
-as a function of depth	X	X	X	X	X	X	X	X
-continuously distributed in space	-	-	-	-	-	-	-	-
-as average at selected points or cells	X	X	X	X	X	-	X	X
-profiles at selected points over time	X	X	X	X	X	-	X	X

Table 1B.

Features of major public domain numerical transport and fate models (continued), from van der Heijde et al. 1988.

Model Characteristics	TRIPM	CFEST	FWEA/ FEMA	HST3D	MOD USGS2D Transp.	MOC DENSE	MOC NRC	RWSTM
<u>Soil/Rock Characteristics</u>								
Confined aquifers	X	X	X	X	X	X	X	X
Aquitards	X	X	-	X	-	-	-	-
Watertable aquifers	X	X	X	X	-	-	X	X
Multiple aquifers	X	X	-	-	-	-	-	-
Heterogeneous	X	X	X	X	X	X	X	X
Anisotropic	X	X	X	X	X	X	X	X
Fractured	-	-	-	-	-	-	-	-
Single soil layer	X	-	-	-	-	-	-	-
Layered soils	X	-	-	-	-	-	-	-
Matrix deformation	-	-	-	-	-	-	-	-
<u>Fluid Conditions</u>								
Single fluid	X	X	X	X	X	-	X	X
Multiple fluids	-	-	-	-	-	X	-	-
Miscible	-	-	-	-	-	-	-	-
Immiscible	-	-	-	-	-	X	-	-
Freshwater	-	-	-	-	-	X	-	-
Salt water	-	-	-	-	-	X	-	-
NAPL ²	-	-	-	-	-	-	-	-
Gas/air	-	-	-	-	-	-	-	-
Varying density	-	-	-	X	-	X	-	-
<u>Flow Conditions</u>								
Saturated	X	X	X	X	X	X	X	X
Unsaturated	X	-	-	-	-	-	-	-
Steady state	X	X	X	X	X	X	X	X
Transient	X	X	X	X	X	X	X	X
<u>Geometry</u>								
1-Dimensional								
-Horizontal								
(vertically averaged)	-	-	-	-	-	-	-	-
-Vertical								
(cross-sectional)	-	-	-	-	-	-	-	-
2-Dimensional								
-Horizontal	-	X	X	-	X	X	X	X
-Vertical	X	X	-	-	X	X	X	-
3-Dimensional	-	X	-	X	-	-	-	-

²Non-Aqueous Phase Liquids

Table 1B (continued).

Model Characteristics	TRIPM	CFEST	FWEA/ FEMA	HST3D	MOD USGS2D Transp.	MOC DENSE	MOC NRC	RWSTM
<u>Transport and Fate Processes</u>								
Advection	X	X	X	X	X	X	X	X
Dispersion	X	X	X	X	X	X	X	X
Matrix diffusion	-	-	-	-	-	-	-	-
Retardation	X	X	X	X	X	-	X	X
Non-lin. adsorption/ desorption	-	-	-	X	X	-	X	-
Ion exchange	-	-	-	-	-	-	-	-
Biotransformation/ degradation	-	-	-	-	-	-	-	-
First-order radioactive/ (bio-)chemical decay	X	X	X	X	X	-	X	X
Chemical reactions/ hydrolysis	-	-	-	-	-	-	-	-
Complexation	-	-	-	-	-	-	-	-
Volatilization	-	-	-	-	-	-	-	-
Heat/energy transport	-	X	-	X	-	-	-	-
<u>Boundary/Source Characteristics</u>								
Point source	X	X	X	X	X	X	X	X
Line source	X	X	X	X	X	X	X	X
Limited area or volume source	-	X	X	X	X	X	X	X
Areally distributed source	-	X	X	X	-	-	-	X
Specified source rate	X	X	X	X	X	X	X	X
Specified concentrations (or concentration function)	X	X	X	X	X	X	X	X
<u>Capabilities</u>								
Contaminant mass/rate of release to groundwater from unsaturated zone	X	-	-	-	-	-	-	-
Contaminant plume extent	-	X	X	X	X	X	X	X
Contaminant concentrations								
-as a function of distance from source	X	X	X	X	X	X	X	X
-as a function of depth	X	X	-	X	X	-	X	-
-continuously distributed in space	-	-	-	-	-	-	-	-
-as average at selected points or cells	X	X	X	X	X	X	X	X
-profiles at selected points over time	X	X	X	X	X	X	X	X

Table 1C.
Features of major public domain numerical transport and fate
models (continued), from van der Heijde et al. 1988.

Model Characteristics	SWENT	SWIFT-II	TRACR3D	TRAFRAP/WT	BIOPLUME-II
<u>Soil/Rock Characteristics</u>					
Confined aquifers	X	X	X	X	X
Aquitards	X	X	X	-	-
Watertable aquifers	-	X	-	X	-
Multiple aquifers	X	X	X	-	-
Heterogeneous	X	X	X	X	X
Anisotropic	X	X	X	X	X
Fractured	-	X	X	X	-
Single soil layer	-	-	-	-	-
Layered soils	-	-	-	-	-
Matrix deformation	-	-	X	-	-
<u>Fluid Conditions</u>					
Single fluid	X	X	X	X	X
Multiple fluids	-	-	X	-	-
Miscible	-	-	X	-	-
Immiscible	-	-	X	-	-
Freshwater	-	-	X	-	-
Salt water	-	-	-	-	-
NAPL ³	-	-	-	-	-
Gas/air	-	-	X	-	-
Varying density	X	X	-	-	-
<u>Flow Conditions</u>					
Saturated	X	X	X	X	X
Unsaturated	-	-	X	-	-
Steady state	X	X	X	X	X
Transient	X	X	X	X	X
<u>Geometry</u>					
1-Dimensional					
-Horizontal					
(vertically averaged)	-	-	-	X	-
-Vertical					
(cross-sectional)	-	-	-	X	-
2-Dimensional					
-Horizontal	X	X	-	X	X
-Vertical	X	X	-	X	-
3-Dimensional	X	X	X	-	-

³Non-Aqueous Phase Liquids

Table 1C (continued).

Model Characteristics	SWENT	SWIFT-II	TRACR3D	TRAFRAP/WT	BIOPLUME-II
<u>Transport and Fate Processes</u>					
Advection	X	X	X	X	X
Dispersion	X	X	X	X	X
Matrix diffusion	-	X	X	X	-
Retardation	X	X	X	X	X
Non-lin. adsorption/ desorption	-	X	-	-	X
Ion exchange	-	X	-	-	-
Biotransformation/ degradation	-	X	-	-	X
First-order radioactive/ (bio-)chemical decay	X	X	X	X	X
Chemical reactions/ hydrolysis	-	X	-	-	-
Complexation	-	-	-	-	-
Volatilization	-	-	-	-	-
Heat/energy transport	X	X	-	X	-
<u>Boundary/Source Characteristics</u>					
Point source	X	X	X	X	X
Line source	X	X	X	X	X
Limited area or volume source	X	X	X	X	X
Areal distributed source	X	X	X	X	-
Specified source rate	X	X	X	X	X
Specified concentrations (or concentration function)	X	X	X	X	X
<u>Capabilities</u>					
Contaminant mass/rate of release to groundwater from unsaturated zone	-	-	X	-	-
Contaminant plume extent	X	X	X	X	X
Contaminant concentrations					
-as a function of distance from source	X	X	X	X	X
-as a function of depth	X	X	X	X	X
-continuously distributed in space	-	-	-	-	-
-as average at selected points or cells	X	X	X	X	X
-profiles at selected points over time	X	X	X	X	X

STATE OF THE ART OF EXISTING NUMERICAL GROUNDWATER QUALITY MODELS OF THE SATURATED ZONE AND EXPERIENCE WITH THEIR APPLICATION IN AGRICULTURAL PROBLEMS

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SCOPE OF REVIEW AND TYPES OF PROBLEMS REQUIRING MODELS

The scope of this review is the practical applicability of water quality modeling of the saturated zone for nonpoint pollution sources due to agricultural activities. Specificity requires the identification of pollutants. The examples focus on nitrate, techniques for pesticides being comparable. The major tasks in which a model of the transport of pollutants and of their transformation in the saturated zone can be applied are:

- (1) interpretation of measured concentration data
- (2) understanding of mechanisms of transport
- (3) understanding of geochemical and microbiological reactions
- (4) estimation of pollutant degradation rates
- (5) identification of major pollutant sources
- (6) predictions of future concentration distributions
- (7) establishment of pollutant balances
- (8) determination of management schemes
- (9) planning of remedial action
- (10) planning of preventive action
- (11) determination of standards and policies
- (12) planning of monitoring programs.

Transport models of the saturated aquifer zone have been applied in numerous pollution cases involving point sources of non-agricultural chemicals. Up to now only few applications in the agricultural field exist in Europe and Australia. The reasons are twofold. On one hand agricultural groundwater pollution is only recently becoming a serious problem in Europe. Secondly, the modeling of agrochemical transport in groundwater combines the complexities of usual pollutant transfer in the aquifer with the difficulties of a little-known, spatially- and temporally-distributed source function.

AVAILABLE TYPES OF MODELS AND EXISTING MODELING EFFORTS

The saturated zone transport models for nonpoint agricultural sources do not differ from the transport models for point sources as far as the model techniques are concerned. The major difference between applications to industrial and agricultural groundwater problems stems from the fact that in industrial pollution cases there is one clearly distinguishable plume from a known source of relatively small areal extent, while in agricultural nitrate modeling areal distributions with relatively small concentration contrasts are analyzed.

The basis for any model is the balance equation in its differential form. The classification of models can be according to

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- (1) processes covered
- (2) dimensionality
- (3) numerical technique used.

Processes modeled usually include advection, dispersion, diffusion, adsorption and chemical transformation. Advection is defined as the bulk motion with the average saturated water flow, while dispersion summarily describes all deviations from average motion on a scale smaller than the scale resolved by the advection term. Dispersion and diffusion manifest themselves as processes which lead to transverse and longitudinal spreading of an initial concentration distribution. Adsorption exerts a delaying influence. Chemical transformations lead to attenuation of the original concentration distribution.

All transport models require as a basis a model of saturated water flow or a discretized regional water balance. A flow model in itself can already be used for the solution of a class of problems encountered in management. It gives directions of average pollutant movement, average path lines, average arrival times, isochrones and catchment boundaries. An example is shown in figure 1, where a horizontally two-dimensional flow model is used to determine catchment area and pathlines to a well-field for a given mode of well operation. The flow model essentially gives the average transport if mixing by diffusion-dispersion is neglected. Homogeneous chemical reactions can be incorporated as functions of time along pathlines.

Zero-Dimensional Models

The most basic model of a catchment of a well or a spring is the zero-dimensional model (e.g. Mercado 1976, Thiery 1984, Strebel et al. 1985). It approximates the catchment or a well-defined part of the catchment as one single or several well-stirred vessels. It is able to describe temporal changes of concentrations at the well as a function of gradually-varying inputs to the catchment which are fairly homogeneously distributed in space. It should always be the first step in a pollutant balance calculation. The size and shape of the catchment or the fluxes into the balance element chosen must be determined by means of a flow model.

On the basis of a known catchment, a zero-dimensional model calculates a balance of inputs and outputs. Figure 2 shows the scheme of a model by Thiery (1984). The aquifer is represented by two cells: one which contains a fast-moving, mobile fraction of nitrate, while the second contains a

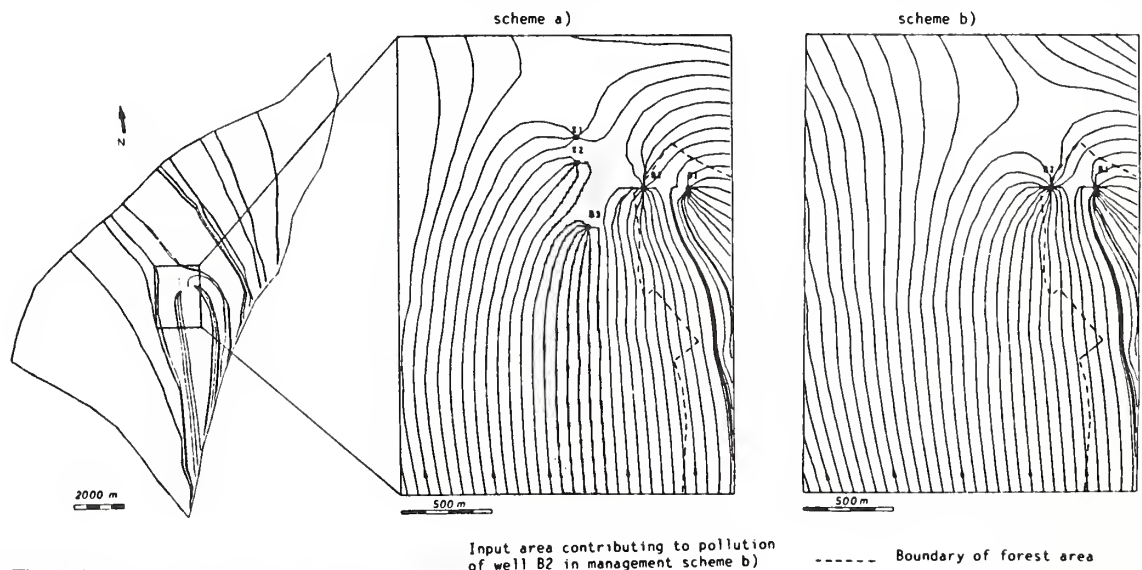


Figure 1.
Application of a horizontally two-dimensional flow model for the determination of catchment area and pathlines (Kinzelbach et al. 1987).

slowly-moving, relatively immobile nitrate fraction in the aquifer. Inputs to the saturated aquifer zone enter the mobile compartment. Nitrate can be delayed by exchange with the immobile compartment. The model results are concentration histories at the well or spring. Simulation results from the Thiery model for a catchment area in France are shown in figure 3. Even such crude approaches as the zero-dimensional balance can be of help in policy evaluation. Once calibrated, the model can be used to analyze the concentration development at a well as a function of future variations in agricultural management.

The balance model - and every saturated zone transport model - requires as input the nitrate flux into the saturated zone. It must be provided from other models which estimate the washout from the root zone and the attenuation in the unsaturated zone. Losses by chemical transformation are not known a priori. They can be estimated if they are the only missing term in the balance equation.

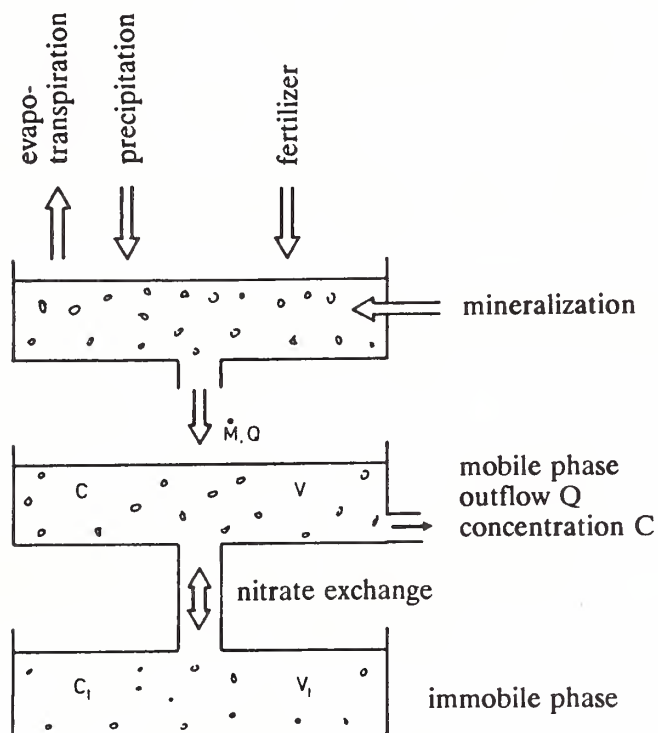


Figure 2.
Schematic description of a two-cell aquifer model for nitrate balancing (Thiery 1984).

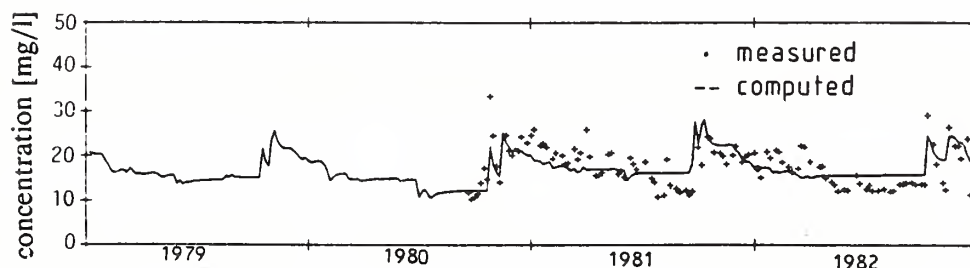


Figure 3.
Calibration results of a two-cell aquifer model (Thiery 1984).

A generalization of the zero-dimensional model is the multi-box or mixing-cell model. Increasing the number of boxes eventually leads to a full-fledged finite difference or finite element model.

Horizontally Two-Dimensional Models

A horizontally two-dimensional model accounts for the superposition of spatially- and temporarily-varying inputs and their effect on drinking water wells. It allows the calculation of concentration distributions averaged over the saturated aquifer depth, as well as concentration histories at pumping wells or observation points. It also allows evaluation of the influence of any input into the flow field on the concentrations in wells. It is a tool for regional management.

Figure 4 shows an application of a horizontally two-dimensional transport model to a problem area in the Upper Rhine valley (Kinzelbach et al. 1987). The model was used for the analysis of observed fast increases in nitrate levels at the wells. As past nitrate inputs were not known explicitly, the model could only be applied for the crude testing of hypotheses. The increase of concentrations in wells K1 and K2 was traced back to inputs due to the conversion of meadows into farmland upstream of these wells. These inputs form a clear plume structure towards wells K1 and K2. The whole area has a generally high nitrate level due to heavily-fertilized asparagus fields. In contrast to other crops asparagus is grown in the same location for many years. This leads to nitrate plumes downstream of asparagus fields, as can be seen south of wells B4 and B3. The nitrate losses by denitrification are negligible except under the forested area on the western edge of the modeled area where a transformation of nitrate takes place with pyrite being turned into sulfate. For the testing of hypotheses, both the knowledge of the flow field and the knowledge of chemical parameters (in addition to the concentrations of nitrate) were necessary. The flow field allows each well to be linked to the area from which its water quality may be influenced. The composition of the water at the wells on the other hand allows identification of different causes for increases in nitrate. For example, nitrate input from underplowing of pasture land is linked to a simultaneous input of chlorides, while a breakthrough of nitrate due to reduced denitrification would be accompanied by a decrease in bicarbonate. The consideration of both flow field and a broad range of chemical parameters also leads to decreased uncertainty in results if flow field information and chemical information support each other.

Vertically Two-Dimensional Models

Vertically two-dimensional models can be applied in agriculture-related transport problems because the horizontal gradients of nitrate or pesticides are usually small. The main objective of vertically two-dimensional transport models is the evaluation of vertical transport and vertical mixing, the interpretation of vertical concentration profiles and the chemical development of a pollutant input in all cases where vertical averaging leads to erroneous results. Figure 5 shows a situation where the distribution of nitrate inputs in the horizontal direction leads to typical vertical profiles of nitrate concentrations which can be traced back to pronounced sources. Inversely, a model calculation could help in tracing a maximum in a vertical nitrate profile back to the source. This type of model has been applied in several locations in Germany.

Figure 6 (Obermann 1981) shows the catchment area of a water works in northern Germany. The vertical cross-section along a streamline was further analyzed by means of a vertically two-dimensional flow model (figure 7). The model allowed the computation of path-lines, travel-times and isochrones. The latter could be compared with results from tritium measurements.

In a nitrate study of the Fuhrberger Feld near Hannover, Böttcher et al. (1985) carried out a comparable study which used more dense information on the vertical distributions of nitrate, sulfate, and tritium.

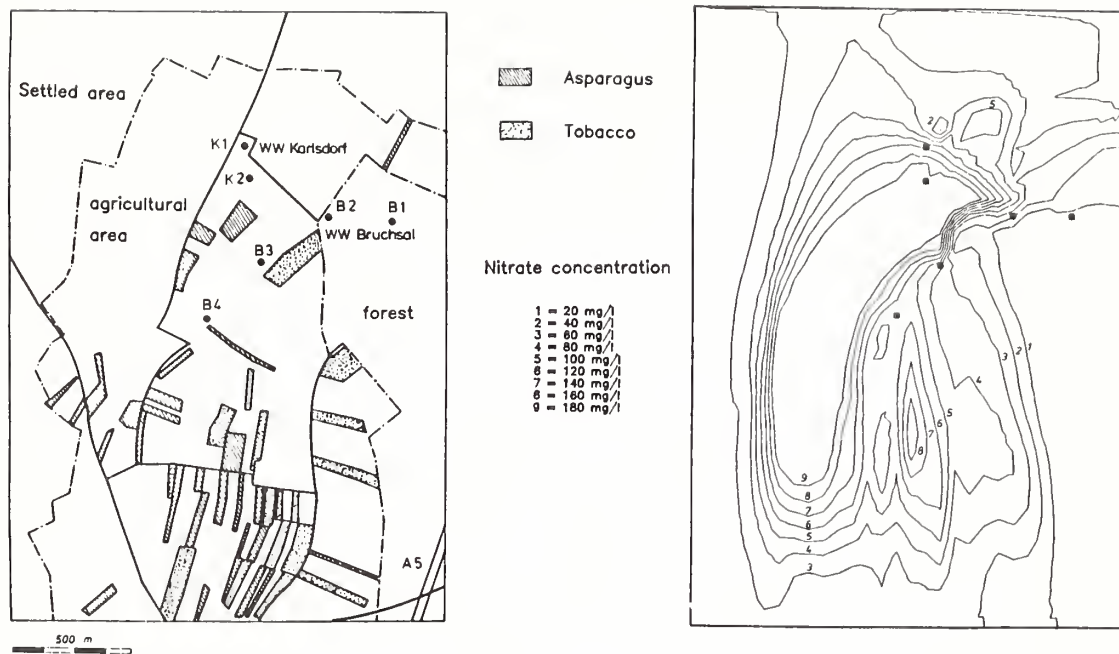


Figure 4.
Application of a horizontally two-dimensional transport model to the interpretation of nitrate concentrations in an intensively farmed region (Kinzelbach and Kauffmann, 1987).

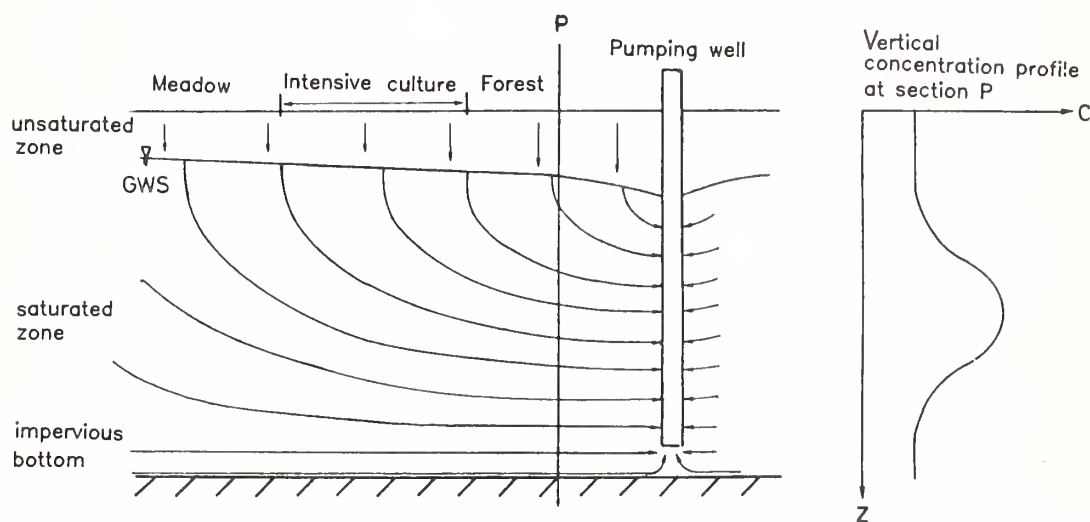


Figure 5.
Schematic description of a typical situation requiring a vertically two-dimensional model.

It should be noted that the accuracy of a back-calculation from a profile to the source depends strongly on the accuracy with which the fluxes of groundwater recharge and the permeability structure of the underground are known. It is doubtful whether the identification of a source by this method is conclusive enough to serve as a legal means.

Three-Dimensional Models

Three-dimensional transport models (to the knowledge of the authors) have not been applied to agriculture-related pollution problems either in Europe or in Australia. Some ongoing research

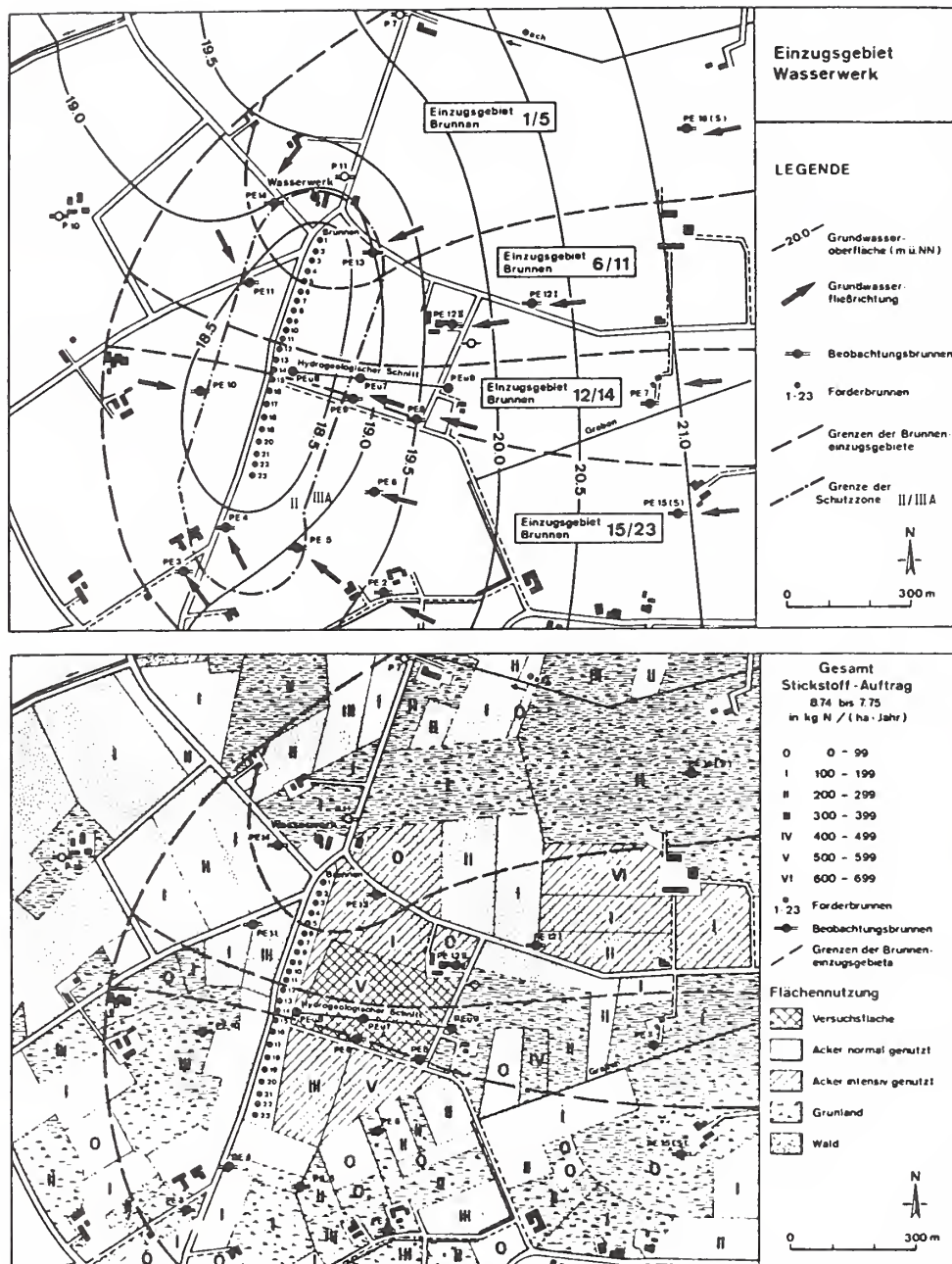


Figure 6.
Horizontal view of a groundwater flow field and surface utilization in the vicinity of Mussum water works (Obermann, 1981).

projects in Germany and Denmark intend to fill this gap. The need is evident in very local problems where the three-dimensional nature of the flow field cannot be neglected, such as in the design of remedial inducement of denitrification by *in-situ* measures in an aquifer. Also in large-scale field problems where the flow field could be viewed as two-dimensional, chemical reactions occurring at varying depths of the aquifer (depending on oxygen concentrations) necessitate a resolution of the vertical aquifer dimension (figure 8).

A three-dimensional model imposes serious demands on the computer which are not easily fulfilled, even with present computers. Still, the problem of computation is more easily solved

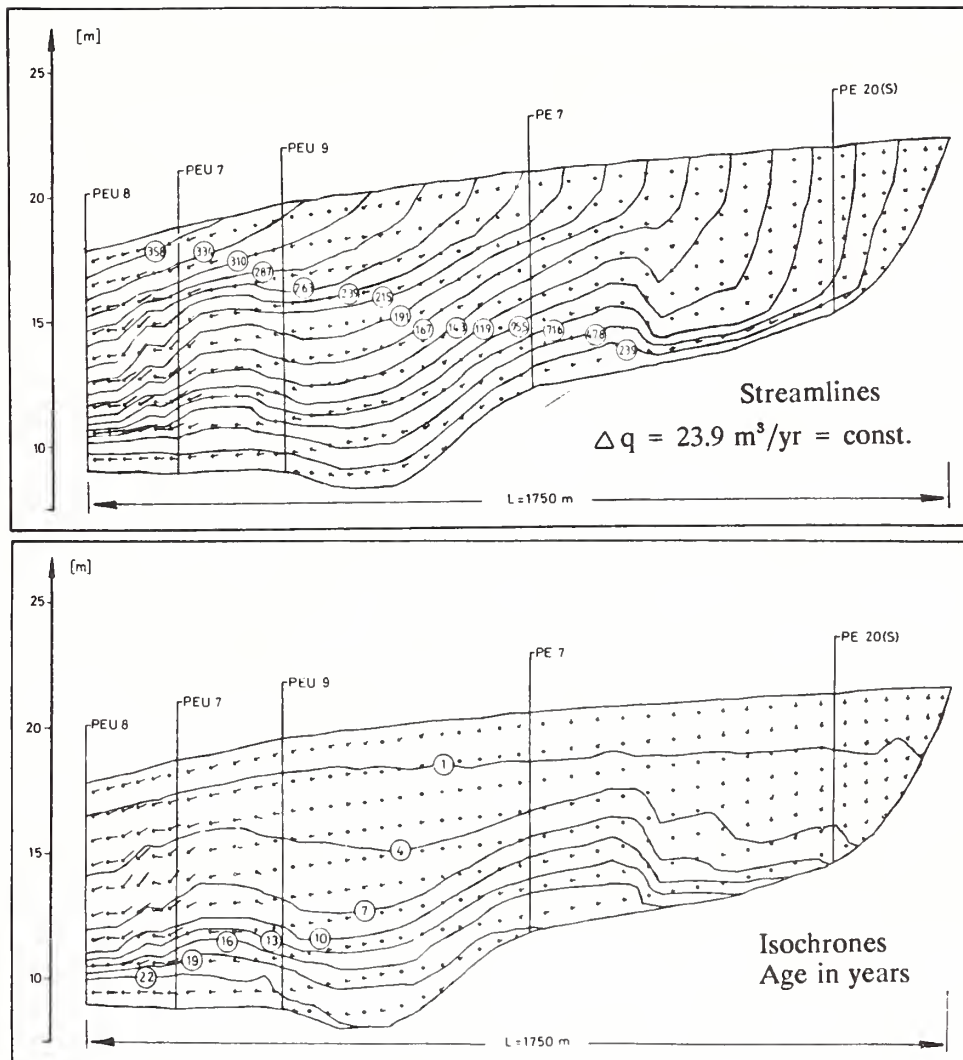


Figure 7.
Isochrones and pathlines in a vertical cross-section through the catchment
of Mussum water works (Obermann, 1981).

than problems posed by the increased requirements in terms of input data, interpretations of output and calibration of parameters. Comprehensive three-dimensional modeling including chemistry and Monte-Carlo simulation to determine model inaccuracy is up to now definitely beyond practical and economic possibilities.

For large-scale problems an interesting and pragmatic model combination consists of a 3-D flow model with a one- or two-dimensional chemical transport model along single stream-tubes or bundles of stream-tubes, the dimensionality of the transport model depending on whether the pollutant source is point-like or distributed (an example related to nitrate transport is given in Bugner (1988)).

METHODS OF SOLUTION

A number of methods are available for the solution of the transport equation. Four types of numerical solution methods have been used in a number of numerical codes. These are

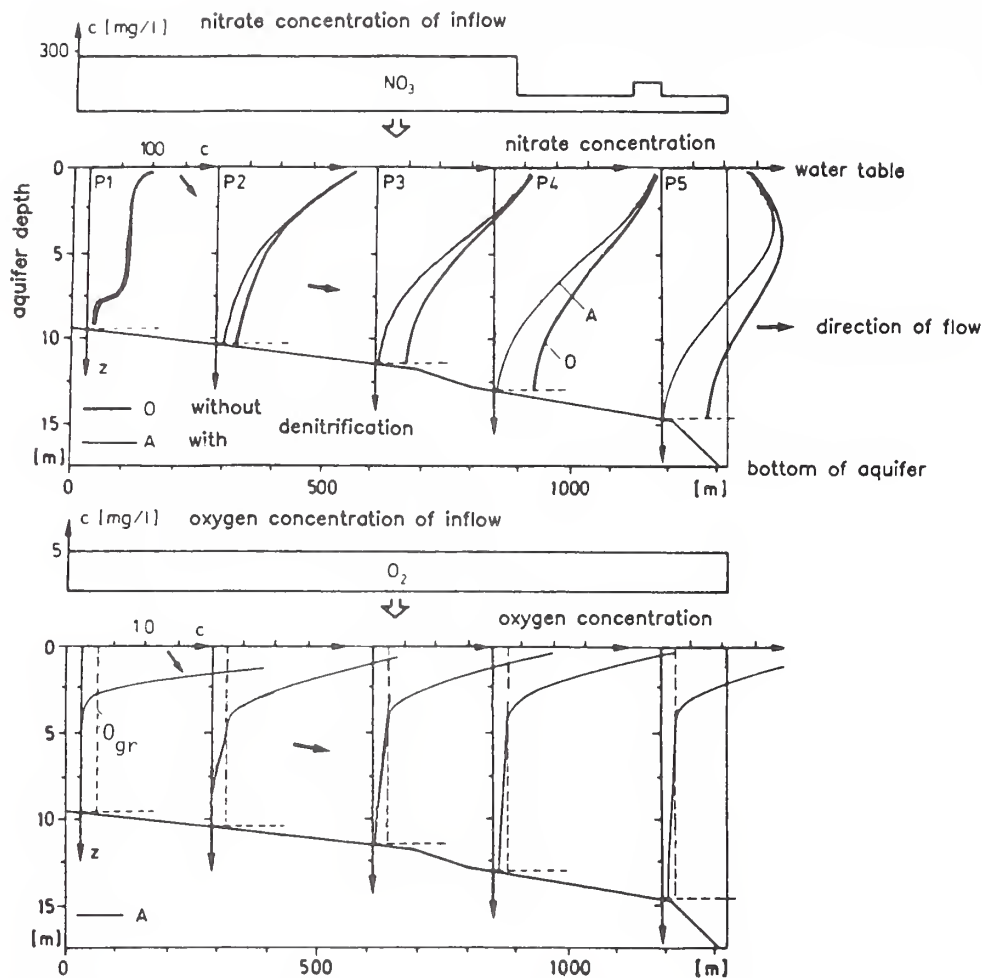


Figure 8.
Simulated chemicals profiles in a vertical cross-section of an aquifer
(Herzer, 1988) (O_{gr} limiting oxygen concentration for denitrification).

- (1) standard finite differences
- (2) standard finite elements
- (3) method of characteristics
- (4) random walk method.

All methods yield satisfactory results provided the limitations of each method are taken into account. For equal accuracy the computational effort may be largely different (Kinzelbach 1987a). Two-dimensional model codes are available in the public domain for all methods. Examples are the finite difference code SWIFT (Dillon et al. 1978), the finite element codes SUTRA (Voss 1984) and SEFTRAN (Huyakorn et al. 1984), the method of characteristics code USGS-MOC (Konikow and Bredehoeft 1978), and the random walk code by Prickett et al. (1981).

Numerical problems encountered in finite difference and finite element methods include numerical oscillations and numerical dispersion. Their application requires a careful planning of the discretization grid to guarantee accurate results. Generally the Courant-number should be less than 1 and the grid-Peclet-number should be less than 2. Yet, for large ratios of longitudinal and transverse dispersivities there may still be important lateral numerical diffusion, which at reasonable spatial discretization size can only be eliminated in finite element models which allow an alignment of element sides and flow direction. This class of models is called principal direction models. They are especially important in vertically two-dimensional modeling where the trans-

verse dispersion effect can be as small as molecular diffusion (Frind, 1982) and where numerical dispersion is particularly detrimental to model results.

In horizontally two-dimensional agricultural applications the task of choosing the correct discretization is on one hand more difficult than in point-source pollution modeling, because the area to be discretized is usually larger than for plumes from point sources. On the other hand, the grid-Peclet-number-criterion can be relaxed in agricultural applications if - as is usually the case - spatial gradients are small.

The method of characteristics and random-walk show their advantages in cases where the discretization requirements of the standard methods cannot be met. The random walk method virtually eliminates both longitudinal and transverse numerical diffusion. In horizontally two-dimensional agricultural applications the random walk method is not efficient. Due to the ubiquitous nature of nitrate, random walk requires particles everywhere in densities which allow a significant evaluation of concentrations. Further, the method is less amenable to the introduction of nontrivial nonlinear chemical expressions. A more detailed comparison of the four basic model types and their properties is presented in Kinzelbach (1987b).

Analytical solutions of the transport equation play only a little role in agricultural applications. Yet, in some cases the advantages of analytical solutions, which combine small computational effort with absence of artificial dispersion, may be exploited. Dillon (1988a) used an analytical model along streamlines in a vertical cross-section through a homogeneous aquifer with a diffuse loading from the top. The model effectively prevents numerical mixing over the vertical. Its results are comparable to the results from the principal direction method (e.g., Frind and Germain 1986). A potential role of analytical models can further be seen in computationally intensive sensitivity calculations.

MODELING OF MACRODISPERSION

The modeling of macrodispersion in the non-asymptotic stage is as yet an unsolved and maybe unsolvable problem. Fickian-dispersion models with constant dispersivities are crude tools in which the dispersivities are mere fitting parameters.

The classical approach to describing the transport of a non-reactive solute by a homogeneous fluid in a porous medium is based on the advection-dispersion differential equation. This equation identifies two transport mechanisms: (1) advection, which represents the transport by the bulk motion of the flowing groundwater and (2) dispersion, which represents the spreading of the solute in the longitudinal and transverse directions relative to the position predicted by the advective movement. This process is related to the flow disturbance exerted by the individual grain particles when viewing the process on a microscopic scale. On a larger scale, dispersion is related to the heterogeneity in the aquifer properties.

Many laboratory experiments have demonstrated that dispersion can be viewed as a Fickian diffusion process with different longitudinal and transverse dispersivities. The verifications have basically been provided by displacement experiments in homogeneous sand-columns of a length on the order of one meter. Such experiments resulted in values of the dispersivity on the order of the grain size.

The good agreement between laboratory measurements and the Fickian-type dispersion theory has motivated the use of this concept also in field problems. This extension, however, is not straightforward, because in the field the geological deposits may be very heterogeneous in contrast to laboratory columns eventually exhibiting rather long-range correlations of inhomogeneities.

Many field tests have been carried out to validate the use of Fickian dispersion theory. A number of tests have been compiled by Gelhar et al. (1985) and the data have been summarized in a figure showing the longitudinal dispersivity as a function of displacement distance (figure 9). The figure reveals two disturbing problems:

- (1) dispersivities observed in the field are orders of magnitude larger than those observed in laboratory experiments; and
- (2) the dispersivity increases with displacement distance. This observation is related to the geological heterogeneity scale, which increases with the scale of the problem.

To interpret these findings, stochastic transport and dispersion theories were formulated (Gelhar et al. 1979, Mathéron and de Marsily 1980, Gelhar and Axness 1983, Dagan 1984). In principle, if the three-dimensional aquifer heterogeneity structure was known in all details, the solute transport could be predicted accurately because the dispersion component would only have to account for the well-understood microscale spreading effect. Such knowledge will never be available in practical field work. Aquifer properties will only be known at a limited number of points and the variation in between is subject to uncertainty due to the unknown, irregular spatial variations. The result of this unknown variation in aquifer properties is modeled as dispersion. The uncertainty of the actual heterogeneity introduces uncertainty into the model predictions.

A rational framework for approaching this problem is provided by interpreting the heterogeneous aquifer properties as random variables characterized by a few statistical parameters. Within this framework, solutions to the flow and transport problem will be expressed in terms of probability distributions. Of particular interest is the mean solution, which provides the expected value of the dependent variable. Further, the solution for the first moment can be used for deriving the effective parameters for large-scale problems. Solutions for the second moment provide quantitative measures of the uncertainty which applies to the mean solution. Such measures of reliability are of highest relevance when interpreting the model results. Any transport model calculation given to decision makers should provide information on its uncertainty. Nowadays, modeling is still far away from this goal.

The mathematical solution to the stochastic transport problem can be approached by different techniques. Gelhar and Axness (1983) apply a perturbation-based spectral representation technique, which provides closed-form solutions for the large-scale parameters and the large-scale variance of the dependent variables. Dagan (1984) uses a particle-tracking Lagrangian approach, which also provides closed-form generic solutions. Using such analytical solution techniques requires a series of assumptions such as infinite extension of the domain, smallness of variations compared to the mean, local statistical homogeneity and the validity of the ergodicity hypothesis. Therefore, their use is limited in field problems; they do, however, provide basic insight into the phenomenon.

By using the above techniques it turns out that the mean large-scale solute transport equation is in fact equivalent to the classical deterministic equation, i.e. macrodispersion can be represented by a concentration-gradient relationship. The dispersivities which enter the mean equation can be calculated from the stochastic theory, and contrary to the microscale equation the macrodispersivity is no longer constant, but increases monotonically with the displacement distance. The theoretical results have shown that the longitudinal dispersivity approaches an asymptotic value, which can be attained after at least 10 correlation scales of the hydraulic conductivity. Both Gelhar and Axness (1983) and Dagan (1984) have shown that the asymptotic value is proportional to the variance of log hydraulic conductivity and the correlation scale, but independent of the microscale dispersion characteristics. The transverse dispersivity is on the other hand affected by the local conditions, but this parameter is in general one or two orders of magnitude less than the longitudinal macrodispersivity. The theoretical findings have been compared with data from field

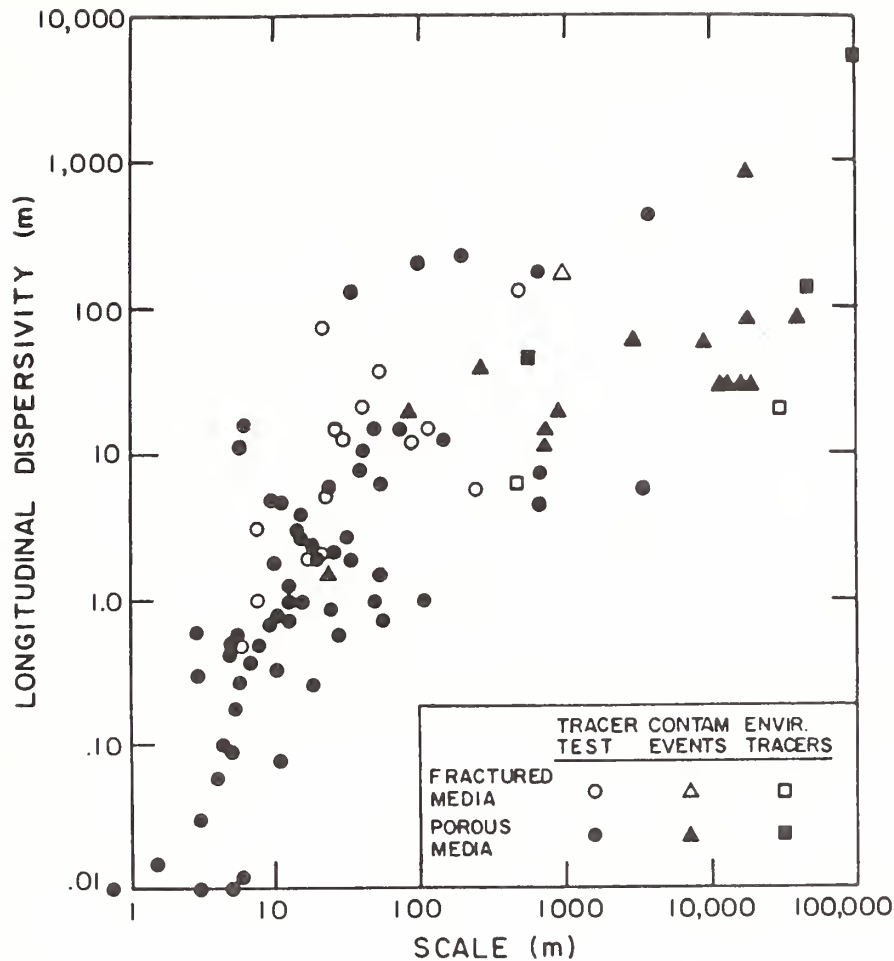


Figure 9.
Scale of observation versus longitudinal dispersivity for the saturated zone (Gelhar et al. 1985).

experiments, and a good support has been obtained of the asymptotic macrodispersivity, derived from the statistical parameters of the aquifer heterogeneity.

The stochastic problem of groundwater flow and transport can also be analyzed by Monte-Carlo techniques. Such methods are less restrictive in terms of underlying assumptions. They do not require infinite extension of the aquifer nor do they require smallness of the variations of hydraulic conductivity compared to the mean value. But the results are more site-specific and the large number of replicates involved requires significant computational resources. Smith and Schwartz (1980) have used Monte-Carlo techniques to demonstrate the shortcomings of the traditional dispersion concept, and their results have also shown the dependence of the dispersivity on displacement distance (or, alternatively, time). The type of work which comes closest to practical needs is the Monte-Carlo modeling as presented by Gorelik (1987). A pragmatic device of introducing scaling dispersivities into random walk simulations of transport is given by Kinzelbach (1987c). It must, however, be noted that the determination of the statistical properties of an aquifer requires a major effort of aquifer sampling which oftentimes cannot be justified. Further, the odd, unknown highly-pervious or impervious lens makes predictions in the near field very much uncertain.

This result is also obtained formally by Gelhar (1986) for the steady-state case. The paper suggests that for distances less than 10 correlation scales from a source, the coefficient of variation (defined as the ratio of standard deviation and expectation value of concentration) will be near one, and consequently a large variability/uncertainty is present near the source. Hence, transport predictions close to the source based on the macroscopic advection-dispersion equation are highly problematic, due to both a displacement-dependent dispersivity and the large variability of the concentration. Essentially the ergodic hypothesis is not applicable in the near-source region. This has the practical implications that reliable predictions can only be provided for this region if the aquifer properties are measured in detail and introduced into a deterministic model. For the far field, where the ergodic hypothesis applies, the stochastic approach may provide useful results.

In general one should utilize all available hydrogeological information in a deterministic sense, and the predictions should also be conditioned on the available point measurements of the hydraulic conditions and the solute concentrations. All the unknown heterogeneity is most conveniently treated in a stochastic manner. However, the stochastic techniques are still in the developing phase and more field validations are called for before they can be used on a routine basis in practical aquifer contamination problems. Also, it must be remembered that the stochastic approach requires the knowledge of the characteristic properties of the distributions of uncertain input parameters. These can only be obtained by extensive field work. If they cannot be provided the approach becomes doubtful as the quantification of uncertainty in the results rests upon an assumed uncertainty of input parameters.

DATA REQUIREMENTS AND PARAMETER IDENTIFICATION

Flow and transport modeling requires a large amount of data, from groundwater recharge, transmissivities or permeabilities to solute input rates and degradation rates. Usually only few of these are readily available. Some have to be estimated by means of the model and sufficient observation data on heads and concentrations. The usual flow model calibration which may be satisfactory in modeling heads is generally not accurate enough for transport modeling (Kinzelbach and Kauffmann 1987). Therefore the calibration of the flow model must be improved by combining it with the calibration of the transport model. In a first step, the calibration of the flow field could take into account information on average flow directions as given by the axis of a known plume.

The processes in the topsoil and unsaturated zone determine the inputs into the saturated zone. In a saturated-zone model they are summarily contained in the source terms or boundary conditions of the transport equation and either presumed to be known (e.g., by unsaturated zone modeling) or looked upon as model inputs to be estimated by the model. The most severe data problem in agricultural applications is the usually insufficient knowledge of source terms, especially of source terms in the past. Estimation of source terms from observed concentration data is usually not unique and introduces a large amount of uncertainty into the model.

For nitrate studies, the denitrification, net mineralization or immobilization, and volatilization terms are often poorly defined, may vary significantly over an area (particularly in grazed pastures) and vary with time (Lawrence 1983). This produces a nonuniform nitrate loading in space and time at the water table. Thus the source term is still the most difficult input term to quantify in many cases.

A new approach has been used recently (Dillon 1988b) to assist the calibration of a model of nitrate leaching from grazed pastures by comparing the variance of the predicted concentration of leached nitrate with the variance of nitrate concentration in groundwater. Mixing within the aquifer demands that the variance of nitrate concentration of groundwater must be less than that of recharge water. This criterion may be used to eliminate otherwise acceptable leaching models (figure 10).

The single largest difficulty in calibrating nonpoint-source models is the lack of systematic spatial contrast in pollutant concentrations. Nonpoint sources are usually quite variable over a region and in statistical terms the variability of pollutant concentrations of groundwater samples within a field at a given depth is often as large as the variability of sample concentrations between fields at the same depth. This implies that a large number of samples are required for statistical tests of differences between means to be valid.

Furthermore due to the expanse of a polluted aquifer, changes with time are usually slow. Resampling of monitoring networks at intervals of twenty years in some cases have failed to reveal a trend with statistical significance (e.g. Aslyng 1986, Dillon 1988b). The calibration of models of pollution due to agricultural activities therefore relies heavily on other forms of information. Point sources such as dairies, saleyards and cheese factories can provide valuable information if their contaminant plumes can be identified. Plumes give marked concentration differences, and if their source history is known, can provide the best evidence for water particle velocities, even if source loads are not well defined (Mazor 1986). Along the same line of argument, pollution plumes from non-agricultural sources can be used for model calibration. In densely-populated countries such as Germany or Denmark coincidence of agricultural and industrial pollution is not rare.

Information on recharge rates from environmental chloride and tritium analyses, or measured groundwater discharge to streams, in conjunction with observed hydraulic gradients provide the most positive identification of hydraulic conductivity on a regional scale.

The occurrence of preferential flow paths at various spatial scales is no more likely to be distinguishable from sample concentrations of the nonpoint pollutant than by detection from piezometry, as the uncertainty attached to random fields of concentrations or hydraulic gradients will tend to mask any deterministic component contained by the handful of observations intercepting such flow paths.

Anisotropy of hydraulic conductivity is a feature which is confounded with vertical mixing coefficients in the case of stratified aquifers. Anisotropy can be determined best near down-gradient boundaries, where the effect of anisotropy on flow trajectories in the vertical plane is most pronounced if vertical mixing is small.

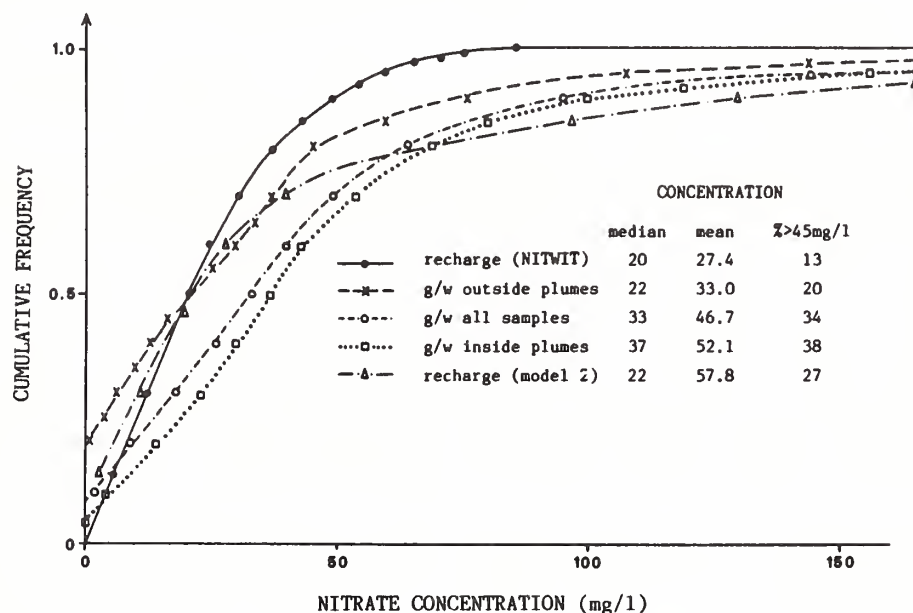


Figure 10. Cumulative frequency of recharge concentration from NITWIT model compared with cumulative frequency of nitrate concentration of groundwater samples.

The longitudinal, lateral and transverse dispersivities are best determined by modeling existing superimposed source plumes. Old sources are preferred, as the scale of the experiment then approaches the scale of the field problem. Without information from point sources or sharp boundaries for nonpoint sources a literature value as from figure 9 provides initial estimates for longitudinal dispersivities in a variety of media. Transverse horizontal and vertical dispersivities are smaller by a factor of 10 to 1000.

For pollutants such as chloride and nitrate it is often assumed that adsorption is negligible. These approximations are thought to be reasonably satisfactory although the opposing effects of anion exclusion and ion-exchange with clay minerals have been observed to affect the transport of chloride in soils.

Identification of parameters describing adsorption are normally derived from batch or column tests. The application of small-scale adsorption results to regional scale problems is thought to be satisfactory for flow in non-fissured media. Adsorption-desorption in dual-porosity media, in a pragmatic approach, is most easily described as a combination of adsorption and an enlarged dispersivity when considering elemental volumes sufficiently large so that preferential paths are described statistically rather than explicitly.

Finally, it must be stressed that uniqueness of model parameters cannot be assured through calibration alone. Therefore all sources of prior knowledge outside of the actual model must be tapped in an attempt at least to rule out certain ranges of parameter values or to reduce ambiguity by constraining parameters to physically reasonable intervals during calibration.

MODELING OF CHEMICAL PROCESSES

Although the concepts and techniques of coupling transport models and chemical models are well known (Rubin 1983) the modeling of chemical processes in aquifer materials remains inherently a complicated task, since the possible number of reaction processes and participating constituents are large. Many reactions have not yet been identified or formulated in quantitative chemical terms. Moreover, if a quantitative theory has been developed, the formulations may turn out to be very complicated and hardly operational, because single reactions cannot be isolated due to the interactions with other processes. In general, any chemical modeling effort of aquifer conditions has a data problem, which is much more serious than that of physical transport modeling. The available field data will usually not allow for even an approximate assessment of the parameters, and since the field modeling experience is limited, a particular application cannot take advantage of other applications.

Some chemical processes have been studied quite extensively in the laboratory by carrying out small-scale batch and column experiments. Such processes include equilibrium-controlled ion exchange, adsorption, complexation and precipitation/dissolution. Equilibrium-controlled reactions apply when reaction rates are much faster than the groundwater flow processes. For these particular reactions and some additional ones, theoretical mathematical frameworks have been developed (e.g. PHREEQUE by Parkhurst et al. 1980) and the parameters entering the equations have shown a consistent behavior on the laboratory scale for various aquifer materials.

Only a few well-documented field applications of geochemical models have been reported, and no conclusive evidence of the predictive capabilities can be provided yet. The major part of the theoretical framework on geochemical modeling developed so far has been related to small-scale, homogeneous soil columns in the laboratory. Transferring these model developments to field conditions is not straightforward because of the natural geological heterogeneity. One may fear that the parameters and relations pertinent to the process are an obvious parallel. It appears that more research should be directed toward developing a theoretical framework that relates results of

laboratory experiments to field conditions, instead of adding still more refinements to the small-scale description of equilibrium-controlled reactions. Garabedian (1987) has applied a stochastic approach to large-scale reactive transport, and more developments along these lines and toward the concept of effective parameters are required (Gelhar 1986).

For reactions involving agricultural pollutants (nitrate and pesticides), the state of modeling is even less satisfactory than for geogenous compounds. All processes mediated by microorganisms present the common problem of transferability of constants. The major phenomenon of interest in the nitrate field is denitrification. It requires anaerobic conditions. Under aerobic conditions nitrate can be considered a conservative tracer. Two major processes of denitrification are distinguished. In the first case organic carbon in the ground serves as a substrate and the oxygen from nitrate serves as an energy source. In the second case, mediated by *Thiobacillus denitrificans*, pyrite in the underground is oxidized to sulfate using the oxygen from nitrate. Both processes are observed in aquifers in Germany (Obermann 1981, Kölle et al. 1985, Rohmann and Sontheimer 1984).

Reaction terms may be time- and space-dependent. It is speculated that in certain watersheds the long-term denitrification has depleted organic carbon and has led to a nitrate breakthrough (Obermann 1981). Aslyng (1986) describes one of the effects of groundwater extraction as lowering water tables from within to below a top soil layer containing organic carbon. Consequently anaerobic bacteria are denied the opportunity to denitrify nitrate-rich groundwater and this nitrate sink term is lost.

Kinzelbach et al. (1989) propose a denitrification model which takes into account a microbial biofilm on the grains and oxygen-controlled denitrification and couples it to a vertically (or horizontally) two-dimensional transport model. Up to now models of this type can only be used for crude hypothesis-testing. Sufficient field data are not available yet and controlled field experiments are strongly recommended.

Chemical transport modeling spans a spectrum from zero-order reaction and first-order reaction to transport of multiple, interacting components. The simple models suffer from the fact that they are not predictive. The reaction rates must in every application be estimated from observation data. The complicated models suffer from the fact that parameters are too numerous and are usually not known in the particular field application. Complicated chemical models will for the foreseeable future be more valuable for conceptualization of the processes in the underground, parameter sensitivity studies and answering fundamental questions than for actual simulation of field problems.

OBSERVATIONS ON LIMITATIONS OF NUMERICAL MODELING

Transport models are crude images of reality. Our knowledge of source and reaction terms, boundary and initial conditions, and the distributed parameters for flow and transport, will never be complete while data acquisition bears a cost. However, measures can be taken to determine the value of model predictions.

Model calibration, using customary trial and error adjustments gives the modeler some "feeling" for the sensitivity of model results to changes in model inputs. A formal sensitivity analysis, centered on the calibrated model parameters, may be used to delineate the range of model predictions for the range of likely values of model parameters.

Stochastic modeling provides a logical extension of sensitivity analysis for uncertain inputs, where their assumed probability distributions are used to generate series of random values used in a Monte-Carlo framework. This provides a suite of model predictions, giving a distribution for the

likelihood of particular consequences arising. It should be emphasized that the uncertainty attached to boundary conditions should also be included in such an analysis. A comprehensive review of the analysis of uncertainty in water-quality modeling is given by Beck (1987).

The ultimate test of model uncertainty is a comprehensive validation of the model on an independent data set, recording discrepancies between predictions and observations. This provides the best information available on model uncertainty as it accounts for all possible failings of a model, from mis-specified processes and boundary conditions, through to the presence of undetected fissures or clay lenses.

However, for regional scale nonpoint-source models, the long persistence of some pollutants in groundwater systems reduces the effectiveness of validation. That is, calibration and validation periods are not independent. Effective validation may therefore require an excitation of the groundwater flow system (e.g., by changes in groundwater extraction patterns), or by some intervention on a regional scale (e.g., suddenly cease the application of a pesticide), to reduce the correlation between calibration and validation periods. Model calibration is most efficient if clear-cut cause/effect relations prevail. These may be induced experimentally in the field by large-scale pumping tests. An example is given in Kinzelbach and Kauffmann (1989).

These difficulties in establishing model uniqueness may often be alleviated as for some parameters there are wide parameter ranges which lead to model predictions having the same consequence for decision making. The decision maker can confidently use an inaccurate model if the recommended course of action is stable despite rather large parameter variations.

CONCLUSIONS AND RECOMMENDATIONS

A wide variety of deterministic transport modeling techniques are available. Therefore there is no major demand for new deterministic transport modeling techniques.

Chemical models are, in principle, available or can be assembled from existing model components. Their application is limited by limited knowledge of parameters and microbiological processes.

Pure flow models can already help in a large number of management problems; however, their calibration should use as much chemical information as possible in order to reduce ambiguity. Methods for the simultaneous calibration of flow and transport are required. As the source term in agricultural transport models is a function of space and time, its unique determination from groundwater concentrations is virtually impossible. Therefore demand exists for methods which allow the simulation of the source term independently from the transport model.

There is a large demand for techniques which give decision makers quantitative information about the uncertainty of model results. The predictive capability of models is limited. This is not due to the lack of modeling techniques, but rather to the limited knowledge of the parameters, data and boundary conditions. Still, there are many applications where modeling is of use. First, a model allows a reproducible interpretation and interpolation of data. Second, even a model of limited accuracy can be used in decision making by worst-case techniques and comparison of alternative courses of action where different tendencies might be reflected more accurately than absolute concentration values. The concepts of stochastic modeling combined with deterministic model techniques may in the future allow to determine both average result and estimates of the intervals in which the true result most probably lies.

Finally, it should be stressed that the art of successful modeling consists to a large degree of identifying interesting questions which under given data constraints can be answered by available modeling techniques with sufficient certainty. There may well be cases where modeling is not

required (because the answer is evident) or not useful (because the uncertainty of results is too large).

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DISCUSSION OF PAPERS PRESENTED IN TECHNICAL SESSION 3, PART 2: GROUNDWATER MODELS FROM THE USER'S PERSPECTIVE

Charles Kinkaid¹, Presiding
Richard Peralta², Recorder

PAPERS DISCUSSED

Groundwater-Quality Models for Planning, Management and Regulation by P.K.M. van der Heijde and T.A. Prickett

State of the Art of Existing Numerical Groundwater Quality Models of the Saturated Zone and Experience with their Application in Agricultural Problems by W.K.H. Kinzelbach, P. Dillon and K.H. Jensen

SPECIFIC QUESTIONS AND COMMENTS

Comment: (Audience) Characteristic time equals total volume divided by flow rate. Since flow rate is computed on the basis of saturated thickness, and a plume may not exist in the entire thickness, this characteristic time is not entirely appropriate.

Response: (W. Kinzelbach, University of Stuttgart, Germany) I agree that this is a problem.

Question: (Audience) How about using natural tracers to get characteristic times?

Response: (W. Kinzelbach) Excellent idea. It is also important to use concentrations in the calibration process. Just because a model is well-calibrated in terms of head, does not mean that it will appropriately simulate future contaminant transport.

Question: (Audience) How can one correctly model contaminants in fractured rocks?

Response: (W. Kinzelbach) One probably can't.

Comment: (Audience) Some people say that appropriate models are relatively applicable regardless of scale.

Response: (T. Prickett, Prickett and Associates, Urbana, Illinois) Scales exist in space and purpose. The scale should be so large that heterogeneity is repeated several times.

Question: (Audience) When collecting data for calibrating a model of a contaminant plume, did your replicates give the same concentration?

Response: (W. Kinzelbach) Yes. If that were not the case, the calibration would fail.

Question: (Audience) If you performed stochastic simulations, what was the variance and stochastic deviation of the results?

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Response: (T. Prickett) Stochastic simulations are generally not performed. Usually one produces results using one's best engineering judgement and also provides a group of answers that are more or less optimistic than that judgement simulation.

Comment: (Audience) Maybe models should be more simple.

Response: (W. Kinzelbach) Some complicated models may be too tough for even a Cray supercomputer. Even if we do use simple models, we need to use spatially distributed data.

Comment: (Audience) Models need to be used for developing management strategies, especially when developing best-management practices (BMP's) for chemical usage.

Response: (Audience) It is practical to do one-dimensional unsaturated zone modeling in developing BMP's. Since some contaminant will probably get to the saturated zone it is important to develop chemicals that do not persist long enough or move far enough to reach the saturated zone. We need improved chemicals and improved models.

SURFACE WATER QUALITY MODELS: MODELER'S PERSPECTIVE

Heinz G. Stefan¹, Robert B. Ambrose, Jr.² and Mark S. Dortch³

ABSTRACT

An overview of process descriptions, assumptions, constraints and other considerations which enter into the development of deterministic mathematical surface water quality models is given in this paper. Modeling of hydrodynamic transport is treated separately for "standing" waters (lakes, reservoirs, ponds, impoundments) and flowing waters (rivers and streams). Some information on sediment transport as it relates to water quality is presented. Models addressing organic wastes and nutrients, synthetic organic chemicals, and metals transport and transformation are addressed in separate sections. The review ends with an outlook toward challenges and possible future developments.

CONCEPTS OF SURFACE WATER QUALITY MODELING

Categories

Surface water quality (WQ) models can be categorized in various ways. One is with reference to their formulation. On that basis we may classify models by the following distinctions:

- (a) Physical vs. mathematical/numerical
- (b) Mechanistic vs. empirical
- (c) Deterministic vs. stochastic
- (d) Steady vs. unsteady state
- (e) Dimensionality (0, 1-D, 2-D, 3-D)
- (f) Hydrodynamic assumptions
- (g) Biogeochemical formulations

This paper deals only with mathematical/numerical, mechanistic, and deterministic surface water quality models. Compilations of available operational surface water models including those that deal with water quality have been given at various times by various organizations in the United States, e.g. by (a) Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis CA (1987); (b) U.S. Geological Survey (Jennings and Yotsokura 1980); (c) Office of Technology Assessment, U.S. Congress (OTA 1982); (d) U.S. Environmental Protection Agency, Center for Water Quality Modeling (1980), Athens, Georgia 30613, (e) U.S. Army Corps of Engineers, Waterways Experiment Station, Vicksburg, MS (1987).

The state of toxicant modeling in surface water was reviewed in 1979 (USEPA 1980) and figure 1 is an example of the systems used. There have been no substantive changes in the concept and/or dimensionality of the models, but the number of recognized pollutant materials and interacting transformations has increased dramatically.

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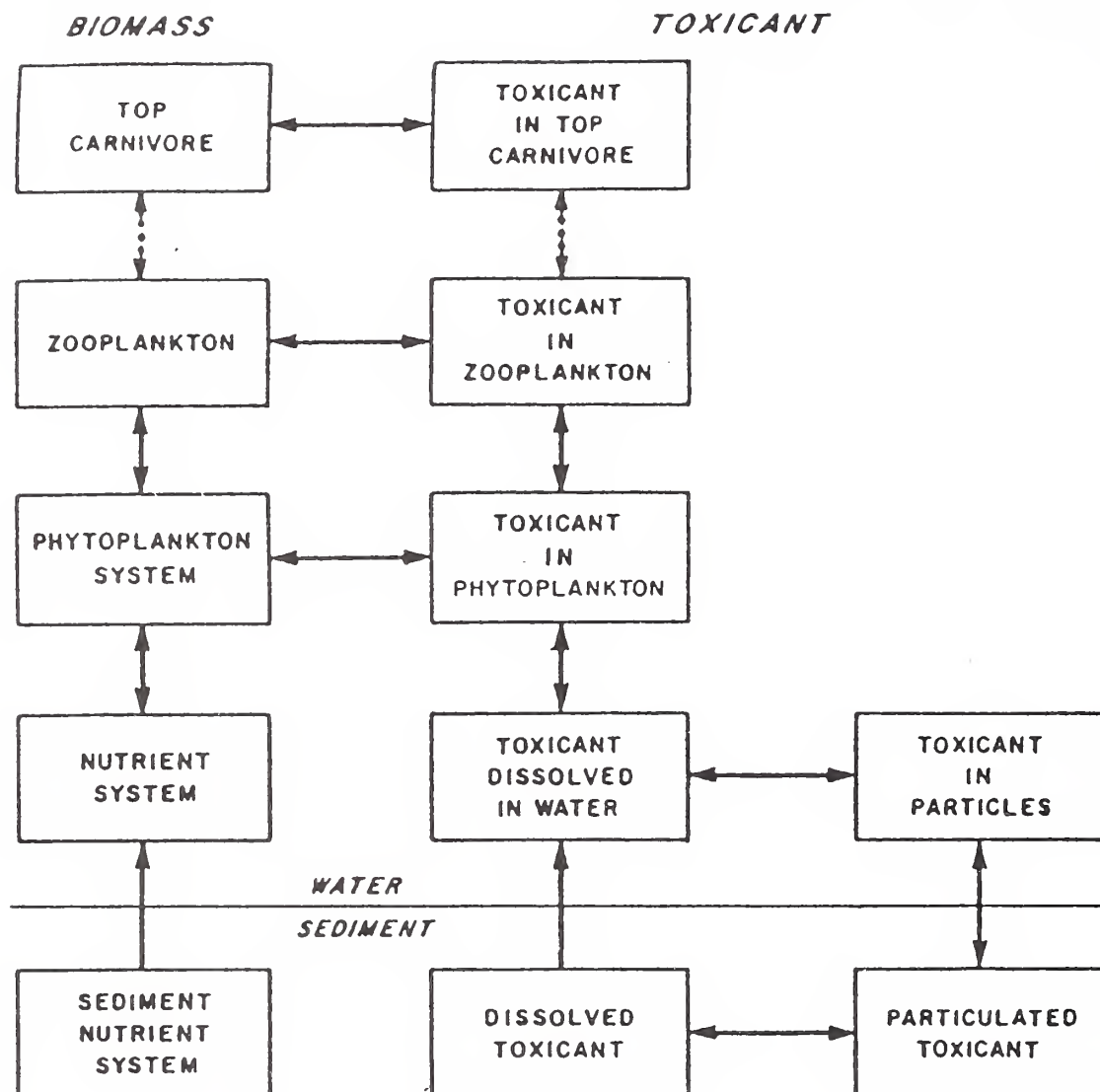


Figure 1.
Systems in toxicant water quality models (from EPA, 1980).

Model Formulation Approach

The classical approach to mechanistic model formulation is to subdivide each water body into a suitable number of control volumes. "Suitable" depends on the purpose of the modeling, the shape and size of the water body, and especially the time scale (years, months, weeks, days or even hours) to be modeled. The time scale influences which physical transport and chemical and biological transformation processes are included in the model. Selection of processes is presently more an art than a science. One rule of thumb is that the shorter the time scale and the larger and more complicated the geometry, the more control volumes will be required. Another rule is to select the longest possible time scale because averaging over long times often makes the model simpler. Science takes over when the basic equations for each control volume are formulated. These equations are transport (conservation) equations for mass of water, and transport/transformation equations for materials in the water. The latter may include expressions

for energy transfer, for chemical equilibrium or chemical kinetics, and for biological kinetics. Water quality parameters which have been modeled include:

- Total dissolved solids, inorganic salts (e.g., Cl^-)
- Inorganic suspended sediments
- Temperature
- Organic wastes and dissolved oxygen
- Bacteria (e.g. *E. coli*)
- Nutrients (e.g. P, N, Si)
- Inorganic carbon (pH)
- Biomass and food chains (e.g. Chl_a , C, zooplankton)
- Metals (e.g., Pb, Hg, Cd)
- Synthetic organic chemicals (e.g. PCB)
- Radioactive materials (e.g. Ra, Pu)
- Herbicides, Insecticides (e.g. dieldrin, DDT)

The classical formulations for nutrient uptake, growth (including photosynthesis), predation, and microbial decomposition are widely used. Recent needs are for models of toxic materials in the form of metals such as Hg, Pb, and Cd; organics such as PCB's, herbicides and insecticides; and for models simulating lowered pH values due to acid rain.

Since one can produce a nearly infinite number of equations, the question to be answered is not "how many equations can I write" but "how many need to be written to solve this problem." The ideal model is the one with the smallest number of equations that can solve the problem.

All models are formulated for a particular purpose. There is no all-purpose model, although models may serve several purposes. The participants in the 1979 workshop (USEPA 1980; Thomann 1982) believed that the formulation of a surface water quality model requires the interaction of three types of people: (a) managers who recognize a water quality problem, (b) specialists who understand or are capable of studying the processes which relate to the problems at hand, and (c) modelers who can synthesize all information pertaining to the problem in mathematical form and solve the resulting mathematical relationships. Only in very simple cases can one person fulfill all three roles.

General steps by which a surface water quality model is developed and put to use are:

- (1) Specify problems, issues, objectives
- (2) Specify theoretical concepts and mathematical relationships (model selection)
- (3) Quantitatively specify parameters/coefficients and boundary conditions
- (4) Calibrate the model
- (5) Verify the model
- (6) Determine model sensitivity, accuracy, validity, and uncertainty
- (7) Apply the model
- (8) Audit the model of the application (Thomann and Mueller 1987).

Conferences on WQ modeling have dealt with: eutrophication (FWPCA 1969; Lorenzen 1979), DeGray Lake (Kennedy and Nix 1987), general issues (Nix and Black 1987; Ott 1976), toxic substances (Jorgensen 1984), and ecological modeling (Jorgensen 1979a).

Parameter values for WQ models must often be developed through field and laboratory studies. Initial estimates may sometimes be found in handbooks (e.g. Jorgensen 1979b). Data sets used for model calibration and validation are usually assembled on a case-by-case basis. A compilation for four rivers, two lakes and one estuary was given by Huber et al. (1984).

In the following sections we shall present some concepts and accomplishments of WQ modeling. Specifically we will address (a) hydrodynamic transport in standing and flowing waters; (b) suspended sediment transport modeling, and sediment/water quality interactions; (c) modeling of organic wastes nutrients and eutrophications; and (d) modeling of transport and transformation of toxic material, including synthetic organics (pesticides) and metals. We will finish with a list of some challenges we perceive for the future and table 1 which shows the more important models discussed in each of the sections of this paper.

WATER QUALITY MODELS FOR STANDING WATERS (RESERVOIRS, PONDS, LAKES)

Approaches

The characteristics of reservoir, lake, or pond water quality models are directly related to the thermo-hydrodynamics in such water bodies that make them substantially different from streams and rivers. In rivers and streams, gravity is the main driving force and bed friction is the main resisting force, resulting in usually very perceptible velocities and a strong tendency to turbulent mixing. Lakes, ponds and reservoirs are often characterized by very slow and weak water movements. The driving forces are from wind shear, solar radiation, heat exchange, and inflows and outflows. Very small density differences caused by temperature gradients from surface heating/cooling and/or by gradients in dissolved or suspended substances (salinity gradients, turbidity) often control the thermo-hydrodynamics of standing waters. Phenomena that are usually absent or can be ignored in river and stream flow analysis are dominant in standing waters. These include stable temperature stratification which hinders vertical turbulent mixing, natural convection caused by unstable density stratification, wind-driven circulation and vertical mixing, density and turbidity currents, and selective withdrawal from density-stratified water. The reader can find overviews of the hydrodynamic features of lakes, reservoirs, impoundments, and ponds in summaries by Mortimer (1974), Wetzel (1975), Gibbs and Shaw (1977), Lerman (1978), Imberger (1979), Csanady (1980), Stefan (1981), Imberger and Hamblin (1982), Harleman (1982), Shanahan and Harleman (1984), Henderson-Sellers (1984), and Annandale (1987).

Hydrodynamics are the basis for many significant differences in ecosystems of lakes/reservoirs and rivers/streams. Lakes often have the longest residence times of water (defined here as total volume of lake divided by total annual outflow). They develop seasonal changes in organisms and chemical processes not affected by the swift motion found in rivers and streams. Storage reservoirs can differ from lakes because of the dominant effects of water level fluctuations and inflow. River impoundments created to make waterways navigable may have fairly constant water levels but highly variable residence time, making them resemble lakes when at low flows, and rivers, when at high flows.

The interactions with the bed also are very different in flowing and standing waters. Slow deposition of fine and organic material on lake/reservoir beds can significantly affect water quality. Equally important can be the release of materials (re-mineralized substances) from the bed due to chemical processes or bacterial decomposition. Bioturbation by invertebrates, or fish, or wind-driven resuspension can contribute greatly to WQ deterioration. In rivers the contributions of such processes are often negligible.

Water quality models of lakes, reservoirs, ponds and impoundments can be formulated as 0-, 1-, 2- or 3-dimensional in space (figure 2). A 0-D model will average concentration over the entire waterbody without allowing variation in space; it will use only one control volume for the entire lake or pond. A 1-D model for standing water usually includes the vertical dimension to account for stratification; thus the model uses a series of horizontal layers. The 2-D models for standing waters are either longitudinal-vertical for density stratified waters or depth integrated in

nonstratified, shallow waters of large horizontal dimensions. In longitudinal-vertical coordinate systems, concentrations are given as $C(x,z)$ where x can be a longitudinal coordinate of a reservoir and z a depth coordinate. Variations in concentration across the width are not treated in such a model and concentrations are assumed averaged with width y . Such a model will require the use of control volumes stacked with depth and length.

Selection of the lowest possible dimensionality, i.e. the smallest number of control volumes (CV) is the most advantageous since a conservation equation must be written for each CV and each water quality constituent. Selection of the dimensionality of a lake, reservoir, pond or impoundment water quality model may be thought to depend mostly on the size of the water body, but it has been shown to be really a function of the purpose of the model. The North American Great Lakes, for example, have been modeled very successfully as completely mixed 0-D continuous flow reactors to develop phosphorus management strategies for eutrophication control (Chapra 1977, Chapra and Reckhow 1983). Lake/reservoir WQ models of different dimensionalities are discussed in the next sections.

0-D Models of Reservoirs, Ponds and Lakes

0-D WQ models of lakes, reservoirs, and ponds contain no information on hydrodynamics other than the hypothesis that the water body is well mixed. They are also referred to as input-output models, box models, etc. The input, I , of a material (nutrient, toxin, etc.) [$MT^{-3}T^{-1}$] and the concentration at time t , $C(t)$, of the material [ML^{-3}] in the well-mixed water body are then related by the conservation equation

$$\frac{dC}{dt} = I - \frac{C}{\theta} \quad [1]$$

which can be solved for various loading functions $I(t)$ and an initial condition $C = C(0)$; t = time; I = the sum of material inflows (a) from all possible sources in the watershed through tributaries, drains, sewers, and overland flow, (b) from the atmosphere, (c) from groundwater, and (d) from internal sources like sediments. The input I is related to the loading L [MT^{-1}] and the lake volume V [L^3] by $I = L/V$. A distinction between nonpoint sources and point sources is common.

The parameter θ is a time constant [T^{-1}]. It sums the rate coefficients of all first-order processes by which the material is removed from the water. These processes may be an outflow Q_0/V or a settling $V_s A/V$, a chemical transformation (reaction) at rate $K_1 C$, or a biological transformation (e.g. bacterial decomposition or zooplankton grazing) at rate $K_2 C$, all in units of $ML^{-3}T^{-1}$. Q_0 is a volumetric outflow rate [L^3T^{-1}], V_s is bulk "settling loss" velocity [LT^{-1}], and A is the surface area of a lake [L^2]. The rate coefficients Q_0/V for outflow, AV_s/V for settling loss, K_1 for chemical, and K_2 for biological transformations are related to the time constant θ in equation 1 by

$$\frac{1}{\theta} = \frac{Q_0}{V} + \frac{V_s A}{V} + K_1 + K_2 \quad [2]$$

If other first order-processes are important, equation 2 can be expanded to include them. It is evident from equation 2 that different residence times differ with compounds (materials) and lakes/reservoirs.

Equations 1 and 2 can be used to quantify not only existing conditions in a lake or reservoir, but also to explore the effects of various alternative management and restoration techniques. For example, a flushing technique can be represented by an increase in Q_0 ; by a reduction in watershed management techniques, diversion, pretreatment, and sediment sealing can be represented by smaller values of I ; dredging or water level rise can be represented by an increase

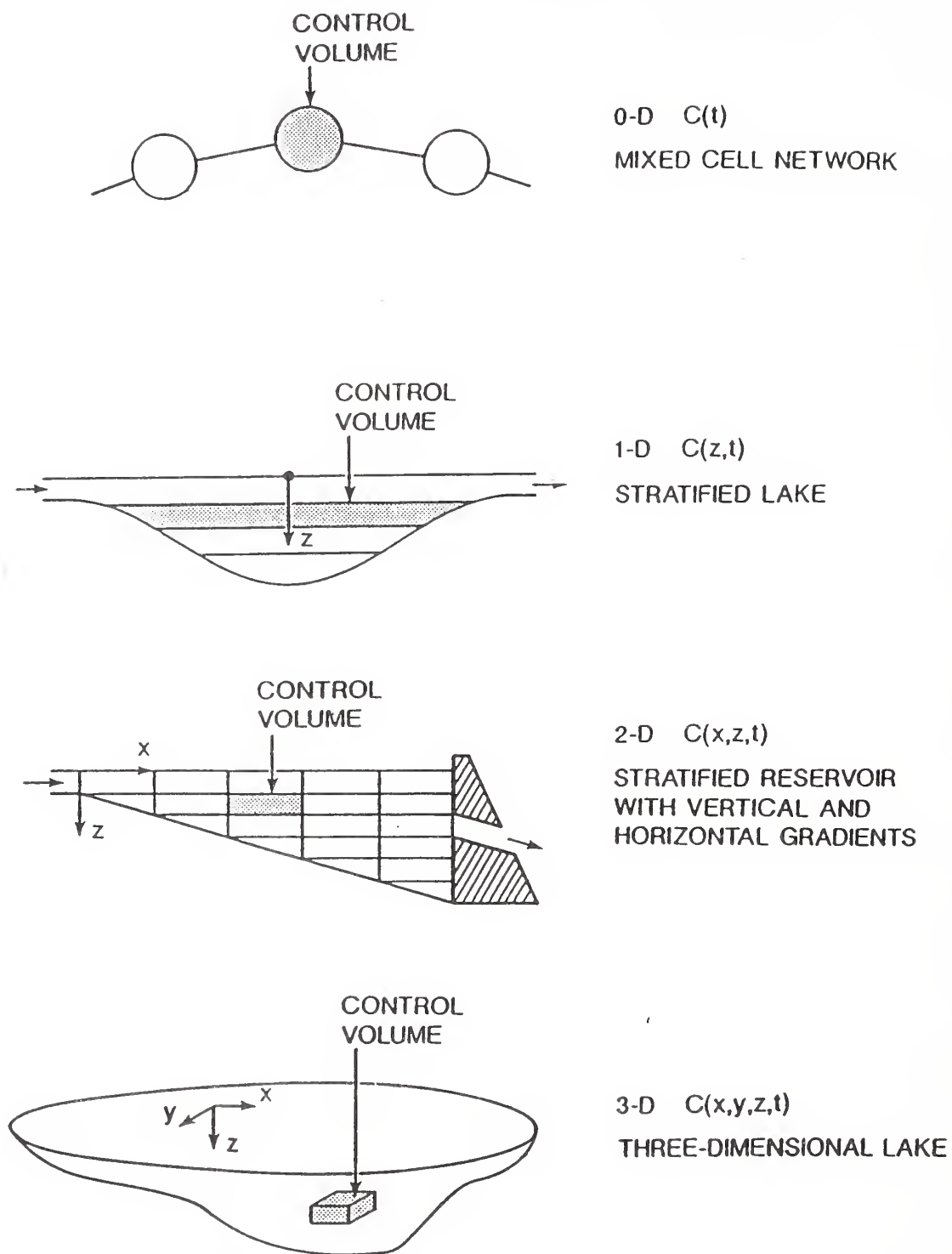


Figure 2.
Dimensionality of lake reservoir models.

in Ψ ; and in-lake treatment by flocculation, chemical treatment, or some form of biomanipulation can be represented by increased values of V_s , K_1 and K_2 , respectively.

0-D models have proved very useful and cost effective for evaluation of long-term effects, measured usually in years. An early, spectacular application was the restoration of Lake Washington and, subsequently, many other applications were made to single lakes (e.g. Sonzogni et al. 1976; Middlebrooks et al. 1974). Failure to recognize important processes in 0-D models (e.g. of material release from the sediments) has led to mispredictions (e.g. of P in eutrophic lakes).

The very well-known Vollenweider (1975), Dillon and Rigler (1974) models for eutrophication control in lakes by P management are extensions of the 0-D models, and can be obtained mainly by adding empirical relationships between P and Chl_a as a measure of biomass concentration, as shown by Chapra and Tarapchak (1976).

0-D models can also be used to simulate series of lakes or lake networks by using the output $C(t)$ of the most upstream lake as input to the next one downstream. An application to the Great Lakes was given by Chapra (1977). It was used to evaluate and predict the effectiveness of several phosphorus management alternatives including P ban in detergents, P removal from municipal sewage by tertiary treatment, and changes in agricultural practices. A summary of the model and its application, is given in Chapra and Reckhow (1983).

The idea has been further extended to interconnected bays and channel systems such as in the coastal plains or in shallow impoundments (Stefan and Anderson 1980a, Demetracopoulos and Stefan 1983). In that case, gravity and wind-driven circulation could be simulated daily or even hourly. Shortening the time scale is essential when flows are highly time variable in response to weather. A model applicable to tidal situations was developed by Schaffranek et al. (1981). 0-D models are also applied to bays connected to larger water bodies (e.g. Chapra 1979). In that case the exchange flow rates (in and out) across the mouth of the bay must be specified based on either tracer observations or hydro-dynamic analysis. Exchange across the mouth of the embayment can be larger than inflow.

1-D Models of Reservoirs, Ponds and Lakes

If water quality variations are to be predicted throughout a season on a monthly, weekly, or even daily scale, internal hydraulics of a lake or reservoir cannot be ignored. Temperature stratification occurs in most "standing waters" in temperate regions, and the associated density stabilities cause vertical gradients in water quality during the summer and winter. 1-D WQ models which describe water temperature, $T(z,t)$, and concentrations, $C(z,t)$, as a function of depth and time are therefore needed (fig. 3). In such models the lake or reservoir is described by a system of horizontal layers, each of which is well mixed. Vertical transport of heat or material compounds between layers is described by a diffusion equation in which a bulk vertical turbulent diffusion coefficient $K_z(z)$ is incorporated in a heat conservation equation of the form

$$A \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(K_z A \frac{\partial T}{\partial z} \right) + \frac{H}{\rho c} \quad [3]$$

where $T(z,t)$ = water temperature as a function of depth z [L] and time [T];
 $A(z)$ = horizontal area of the lake as a function of depth [L^2];
 $H(z,t)$ = internal distribution of heat sources due to radiation absorption inside the water column,
 ρ = water density, and
 c = specific heat.

At the water surface, heat fluxes due to solar radiation, atmospheric radiation, back radiation, evaporation and convection are applied. The expressions used for these fluxes are not presented

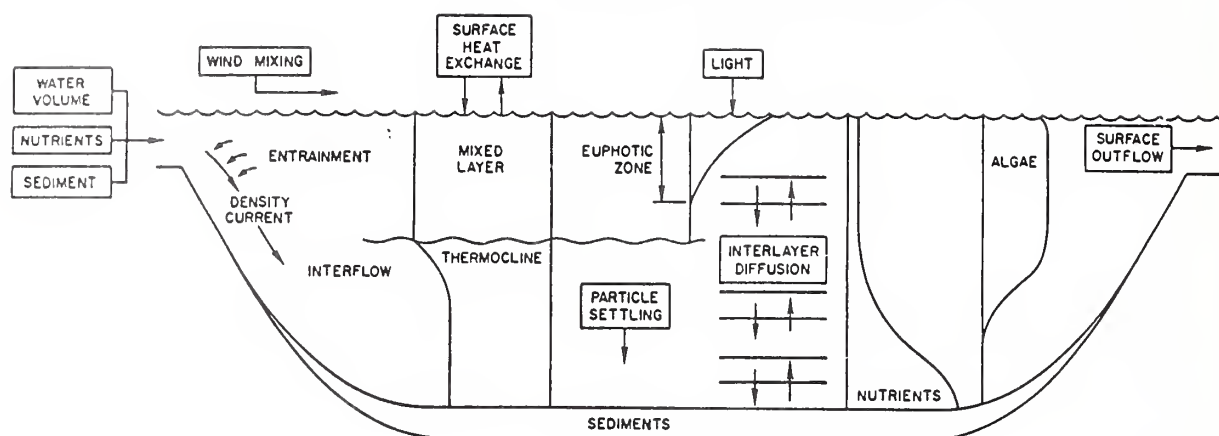


Figure 3.
Schematic representation of the variables and
processes simulated in the 1-D MINLAKE model.

here, but can be found in papers by Edinger et al. (1968, 1974), Ryan et al. (1974), Harleman (1982), and Stefan and Gulliver (1980).

Basically, two methods have been used for computing total net heat transfer at the water surface. In the first method, each of the fluxes is computed and added to form the total net surface heat transfer which is then converted to a rate of temperature change for use in the temperature balance equation. Several of the flux terms are dependent on the water temperature; thus, the most recently computed value for water temperature is used in computing these terms. This approach is referred to as a direct energy balance.

The second method is based on the equilibrium temperature concept, which states that when the water temperature equals the equilibrium temperature, heat exchange does not occur (Edinger et al. 1968). With the water temperature set equal to the equilibrium temperature and with the total net heat transfer set to zero, the flux terms can be expressed in terms of the equilibrium temperature (Edinger et al. 1974); the equilibrium temperature can then be solved iteratively and independently of the thermal simulation. The total net heat transfer becomes the difference in the equilibrium temperature and water temperature times a heat transfer coefficient, which can also be computed prior to the temperature simulation.

Both methods for heat transfer require project location (latitude, longitude, and altitude) and meteorological data (dry bulb temperature, wet bulb or dew point temperature, wind speed, cloud cover, and atmospheric pressure).

The internal heat source $H(z,t)$ is generated by solar radiation which penetrates into the water. The amount of solar radiation absorbed in each layer is approximated by Harleman (1982) as

$$H(z,t) = (1-\beta)(1-r)\phi_s \frac{\partial}{\partial z} (Ae^{-\eta(z_s-z)}) \quad [4]$$

where ϕ_s = solar radiation = $\phi_s(t)$ [L^{-2}];
 r = reflectivity;
 β = surface absorption ($\sim 40\%$);
 η = attenuation coefficient [L^{-1}]; and
 z_s = elevation of water surface [L].

In reservoirs which have inflows and outflows, equation 3 must be expanded (Huber et al. 1972; Orlob and Selna 1970).

$$A \frac{\partial T}{\partial t} + \frac{\partial(Q_v T)}{\partial z} = \frac{\partial}{\partial z} \left(K_z A \frac{\partial T}{\partial z} \right) + B u_i T_i - B u_o T + \frac{H}{\rho c} \quad [5]$$

where u_i and u_o = horizontal inflow and outflow velocities [LT^{-1}];
 B = reservoir width [L] at depth z [L];
 T_i = inflow temperature [$^{\circ}C$];
 Q_v = vertical flow rate [L^3T^{-1}]; and other terms are as previously defined.

To satisfy continuity, Q_v must satisfy

$$Q_v(z,t) = B \int_0^z (u_i - u_o) dz \quad [6]$$

In a 1-D approach, determination of $q_i(z) = B(z)u_i(z)$ may require analysis of density currents through multilayered systems, such as shown by Akiyama and Stefan (1984, 1987). Determination of outflow may require analysis of stratified (selective) withdrawal such as described by Brooks and Koh (1969) and Huber et al. (1972).

If the numerical solution of equations 4 and 5 is done with fixed vertical coordinates such as described by Orlob and Selna (1970) for one of the earliest reservoir models, the computations with a moving free surface become cumbersome. A more recently introduced alternative of a Lagrangian nature keeps track of reservoir volumes in a stack of expandable/contractible layers, and determines the position of those layers by comparing cumulative volume curves for layers to the topography-dependent, lake specific volume characteristic $V(z)$. Examples of this are found in models DYRESM (Imberger and Hamblin 1982), RESQUAL II (Stefan et al. 1982) and CE-QUAL-R1 (Environmental Laboratory 1986a).

The vertical turbulent diffusion coefficient is usually introduced as an empirical function $K_z(\epsilon)$ [L^2T^{-1}] of a density stability parameter ϵ or N^2 [L^{-1}] where

$$\epsilon = \frac{1}{\rho} \frac{d\rho}{dz} \quad \text{and} \quad N^2 = \epsilon g \quad [7]$$

Uncertainty in the K_z values is often large. Attempts to relate K_z not only to stability, which hinders the development of vertical turbulence, but also to the forcing elements, particularly wind, and inflows have been only partially successful. A recent review of this subject has been given by Ford and Johnson (1986). McCormick and Scavia (1981) derived from stability and boundary layer theory an expression

$$K_z = \frac{u_*^3}{\beta g \alpha \left(\frac{\partial T}{\partial z} \right) k^2 z^2} \quad [8]$$

where u_* = wind-induced surface shear velocity = $\sqrt{\tau_w / \rho_a}$ [LT^{-1}];
 β = empirical coefficient [LT^{-1}] = $3.5 \cdot 10^{-4}$ [m^{-1}] for Lake Ontario;
 g = acceleration of gravity [LT^{-2}];
 α = coefficient of thermal expansion [$^{\circ}C^{-1}$];
 k = von Karman constant ~ 0.4 ;
 z = depth below surface [L];

$$\begin{aligned}\tau_w &= \text{wind induced surface shear stress} \sim 0.0015 \rho_a W^2; \\ \rho_a &= \text{air density [ML}^{-3}\text{]; and} \\ W &= \text{wind velocity [LT}^{-1}\text{].}\end{aligned}$$

When thermal instability sets in, natural convection usually produces complete mixing over the range of instability plus a region of penetrative mixing. This high rate of mixing is usually well handled by very high values of $K_z(z)$. An alternative to turbulent vertical diffusion coefficients is the use of k - ϵ closure models (Rodi 1980). This approach was used, for example, to give 1-D vertical temperature distributions in a Vänern, Sweden (Omstedt 1984).

To predict mixed layer depth h [L], an expression of the following form can be used (Stefan and Ford 1975)

$$\frac{1}{2} \frac{dh}{dt} \frac{\Delta \rho g h}{\rho_o u_*^3} \approx \text{Const.} \quad [9]$$

where $\Delta \rho$ = density differential between mixed layer and next adjacent layer below; and u_* = shear velocity due to wind during time interval dt [LT⁻¹].

When the stratification is strong, dissipation becomes important. Therefore equation 9 was extended by Bloss and Harleman (1979).

The transformation and transport of dissolved substances in a 1-D vertically stratified water quality model are described by an equation similar to equation 5.

$$V \frac{\partial C}{\partial t} = -Q_z \frac{\partial C}{\partial z} \Delta z + \frac{\partial}{\partial z} \left[K_z A \frac{\partial C}{\partial z} \right] \Delta z + Q_i C_i - Q_o C \pm S \quad [10]$$

Equations 10 and 5 are equivalent and given by Orlob and Selna (1970) and Huber et al. (1972), respectively. The sink/source term "S" includes chemical and biological transformations and can take many different forms. One of the simplest is a single first-order reaction, $S = K_1 C V$, where K_1 is a rate coefficient [T⁻¹]. For suspended materials a settling term $-(\partial(V_s C A)/\partial z) \Delta z$ must be added to the right-hand side of the equation, where V_s = settling velocity of the particles [LT⁻¹].

Many 1-D water quality models of the kind described exist (Orlob 1983). We are acquainted with CE-QUAL-R1 (Environmental Laboratory 1986a), the Hydrologic Engineering Center HEC5 models (1978), Orlob and Selna's model (1970), Huber et al.'s model (1972), Imberger and Patterson's DYRESM model (Fischer 1981), Stefan et al.'s RESQUAL II (1982) and Riley and Stefan MINLAKE model (1989). Other similar 1-D reservoir models are TVA's RESTEMP (Brown and Shiao 1981) and WRMMS (TVA 1976) models, and a USGS model (House 1981). All of these basically 1-D hydrodynamic models simulate temperature stratification, but CE-QUAL-R1 and MINLAKE also handle a large array of water quality parameters such as dissolved oxygen, algae, nutrients and conservative substances. CE-QUAL-R1 is designed for reservoirs; MINLAKE is intended for lakes. A similar model FARMPOUND for small rural impoundments was developed by the USDA/ARS.

The U.S. Army Corps of Engineers' vertically one-dimensional model CE-QUAL-R1 (Environmental Laboratory 1986a) simulates temperature plus as many as 34 other water quality parameters. Primary physical processes included are surface heat transfer, shortwave and longwave radiation and penetration, convective mixing, wind-and flow-induced mixing, entrainment of ambient water by pumped-storage inflows, inflow density current placement, selective withdrawal, and density stratification as affected by temperature and dissolved and suspended solids. Major chemical and biological processes in CE-QUAL-R1 include: the effects on dissolved oxygen (DO)

of atmospheric exchange, photosynthesis, respiration, organic matter decomposition, nitrification, and chemical oxidation of reduced substances; uptake, excretion, and regeneration of phosphorus and nitrogen and nitrification-denitrification under aerobic and anaerobic conditions; carbon cycling and alkalinity-pH-CO₂ interactions; trophic relationships for phytoplankton and macrophytes; transfers through higher trophic levels (i.e. zooplankton and fish); accumulation and decomposition of detritus and organic sediment; coliform bacteria mortality; and accumulation and reoxidation of manganese, iron, and sulfide when anaerobic conditions prevail.

The U.S. Army Engineer Waterways Experiment Station (WES) has expended considerable effort during the past 20 years to develop a single generalized model for prediction of outflow water quality at dams, building on the work of Brooks and Koh (1969) and many others. Smith et al. (1987) synthesized the various point sink models into a single generalized, point sink model. The WES selective withdrawal models have been coded into a documented program referred to as SELECT (Davis et al. 1987). When used as a stand-alone program, SELECT computes the in-pool vertical distribution of outflow and outflow concentrations of water quality constituents, given the in-pool vertical distribution of water density and water quality constituent concentrations, the outlet configuration and depth, and the discharge rate. In subroutine form, SELECT is used in reservoir water quality models (e.g. CE-QUAL-R1, Environmental Laboratory 1986a) to compute the outflow distribution and release water quality. Numerical hydrodynamic models for stratified flow, such as the WESSEL (Thompson and Bernard 1985) and STREMR (Bernard 1988) codes, can be used as experimental tools to study the withdrawal characteristics of unusual outlet configurations.

2-D Models of Reservoirs, Ponds and Lakes

2-D water quality models were developed for long deep reservoirs in which significant vertical WQ gradients are coupled with horizontal ones. For example Lake Powell and Lake Mead reservoirs on the Colorado River require such an approach. There are a few 2-D models available. One is the LARM model (Laterally Averaged Reservoir Model) developed by Edinger and Buchak (1983) and Buchak and Edinger (1984a, 1984b); another is the COORS (Computation of Reservoir Stratification) model by Waldrop et al. (1980), Harper and Waldrop (1980a, 1980b) and TVA (1986). Both models solve two-dimensional advection/diffusion equations in a vertical longitudinal plane through a reservoir. The models are width integrated. These models can predict the 2-D temperature structure of deep reservoirs throughout the annual stratification cycle and compute temporal and spatial hydrodynamics of reservoirs to provide advective components for water quality models. A later version of LARM referred to as CE-QUAL-W2 (Environmental Laboratory 1986b) has been modified by the Corps of Engineers to include 20 water quality constituents.

Temperatures and velocity gradients of deep storage reservoirs occur primarily in the longitudinal (x) and vertical (z) directions. Lateral (y) contributions of shear stress, continuity, etc., are important, but their effects can be included through an integration procedure. This procedure reduces by one the number of equations and independent variables by eliminating the y-momentum equation and simplifying the remaining equations. Additionally, most vertically stratified hydrodynamic/transport models for reservoirs (and other surface waters) make the hydrostatic assumption, which reduces the vertical equation to a simple pressure gradient relation.

Empirical functions are defined to include the effects of turbulent processes which occur at a scale smaller than the resolution afforded by the solution procedure (i.e. a finite difference grid). The technique chosen in the COORS model is to assume that the effects of turbulence could be incorporated by using Prandtl's mixing length hypothesis where the mixing length is defined by half the vertical spacing between grid planes.

Boundary conditions included in most 2-D models are inflows and outflows (flow rate and temperature must be specified for inflows), bedshear, no heat transfer through the bed, heat flux through the free surface, and surface wind shear. These conditions are similar to those imposed in the 1-D models.

The numerical solution of the equations in the COORS model is explicit and time marching, whereas the water surface solution of the CE-QUAL-W2 model is implicit, so that larger time steps can be taken. Finite differences are used to discretize the equations in both models.

CE-QUAL-W2 consists of directly coupled hydrodynamic and water quality transport models. Hydrodynamic computations are influenced by variable water density caused by temperature, salinity, and dissolved and suspended solids. Developed for reservoirs and narrow, stratified estuaries, CE-QUAL-W2 can handle a branched and/or looped system with flow and/or head boundary conditions. With two dimensions depicted, point and nonpoint loadings can be spatially distributed. Figure 4 is an example of CE-QUAL-W2 applied to D.O. concentration in DeGray Lake. Relative to other two-dimensional models, CE-QUAL-W2 is efficient and cost effective to use.

In addition to temperature, CE-QUAL-W2 simulates as many as 20 other water quality variables. The physical, chemical, biological processes of CE-QUAL-W2 are very similar to those in CE-QUAL-R1 with the following exceptions: it does not include transfer to higher trophic levels of zooplankton and fish; it does not account for substances that are accumulated in the sediments other than organic matter; it only contains one algal group rather than three; it does not include macrophytes; and it does not include the sediment release and oxidation of sulfur and manganese when anaerobic conditions prevail, although it does allow specification (as a boundary condition) of flux from the sediments of iron, ammonia nitrogen, and phosphate phosphorus during anaerobic conditions.

A box model approach to 2-D reservoir modeling was used by Brown (1985). The model, named BETTER for, "Box Exchange Transport Temperature and Ecology of Reservoirs," has been applied to TVA reservoirs. In this model, the reservoir is segmented into an array of volume elements or boxes. These boxes are described with a volume, an upper interface or surface area, and a downstream conveyance area. The BETTER model uses a floating layer scheme, so that the layer boundaries remain at specified depths relative to the surface elevation. The layer spacing is arbitrary and can be changed by the user if vertical gradients are not being adequately reproduced.

In the BETTER model, the flow patterns in the lake or reservoir are modeled as longitudinal and vertical flow transfers between the array of volume elements. Daily flow patterns can be calculated based on the inflow and outflow. The flow patterns are influenced by the temperature patterns. The inflow temperature governs where the inflow will enter the water column, and subsequent flows will move through the reservoir along matched density pathways. In addition to horizontal and vertical flows (transport), vertical mixing (exchange) can be simulated. Mixing may be caused by wind surface cooling, or turbulent flows. Volumetric exchanges between adjacent layers or a diffusive formulation can simulate mixing. A surface mixed layer can be calculated for each day in response to surface cooling and wind mixing.

An introduction to box-type multi-dimensional models was given by Chen and Smith (1979), and a review by Shanahan and Harleman (1984). A 2-D box-type model for water quality has also been used for Lake Erie (Lam et al. 1983).

The most recent developments in 2-D reservoir modeling include (a) the replacement of eddy diffusion coefficients and mixing length theories by other turbulence closures, e.g. $k-\epsilon$ models and (b) the solution of the fundamental, fully convective primitive equations on powerful supercomputers. Examples of this approach have been given by Ni et al. (1985), Farrell and

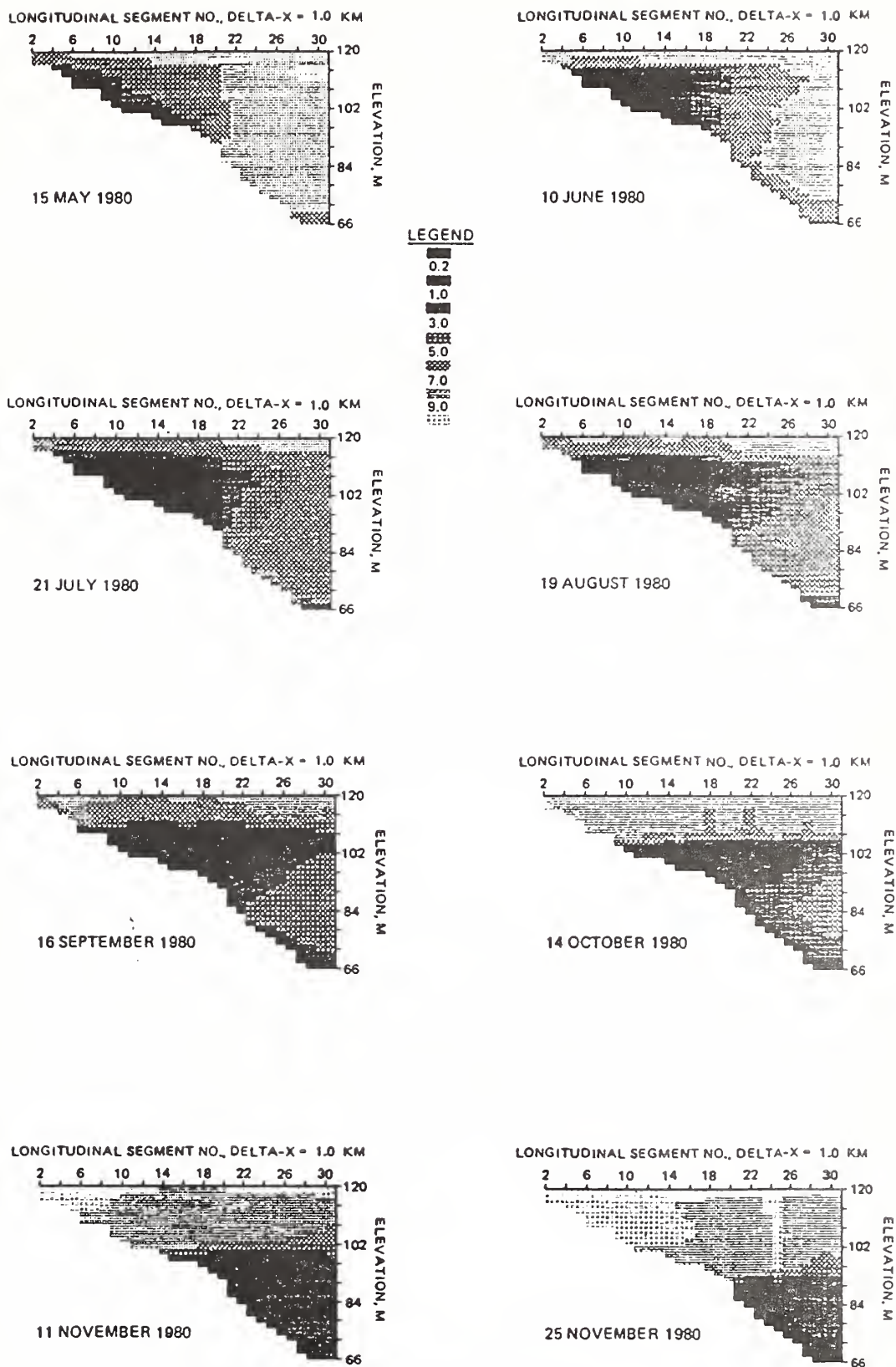


Figure 4.
Shaded contours of predicted D.O. concentration using CE-QUAL-W2
(Martin 1987) DeGray Lake verification simulations (concentrations
milligrams per liter).

Stefan (1986), Sauvaget (1987), and Thompson and Bernard (1985). At this stage of development these models are pure hydrodynamic models. Water temperature (or water density) is the only WQ parameter used.

Selection of a width-integrated x,z -coordinate system in a vertical plane is appropriate for 2-D models of long, deep reservoirs. Depth-integrated models using x,y -coordinates are appropriate for shallow, wide lakes. Liggett developed hydrodynamic depth-integrated models for this purpose. Bennett et al. (1983) describe a typical 2-D lake circulation model. These models are typically driven by windshear and include no stratification effects on vertical turbulence since they are depth integrated. This approach was used to model Lake Balaton in Hungary (van Straten and Somlyódy 1980). Other examples are given by Shanahan and Harleman (1984).

3-D Models Of Reservoirs, Ponds and Lakes

3-D water quality models have not been used extensively because of the computational expense, as well as for other reasons. 3-D flow simulations of lakes and reservoirs have been made by Simons (1973, 1975, 1976), and Leendertse and Liu (1975) and verified in both small and large lakes. A special version was produced by Kielmann and used for pollutant transport in the Baltic Sea (Funkquist and Gidhagen 1984). The model uses seasonally and depth-varied (six layers) eddy viscosities and eddy diffusivities. These models do not overcome the uncertainty in the turbulence closing, but the predicted circulation is a reasonable synthesis of wind-induced and thermocline circulation. The diffusive transport created by turbulence smaller than the grid size in the horizontal (several kilometers) is modeled by a Monte Carlo technique. This means that the calculated turbulent part of the particle velocity is related to the eddy diffusivity in a physically correct way. Some results obtained for the North American Great Lakes have been used in a 3-D WQ model for Lake Ontario (Thomann et al. 1975, 1979). The WQ models are of the multiple box type: multilayered in the vertical, with each layer subdivided into very large elements representative of the coastal regions and the pelagic waters (fig. 5). Advective and dispersive flows between boxes are determined by flow budgets based on long-term observed hydrology. Relying on the NOAA Geophysical Fluid Dynamics Laboratory, researchers at Princeton and Stevens Institute of Technology are compiling a massive 3-D time dependent model of the New York-New Jersey estuary. The Waterways Experiment Station is compiling a similar model for studying eutrophication problems in Chesapeake Bay.

WATER QUALITY MODELS FOR FLOWING WATER (STREAMS AND RIVERS)

Approaches

Water quality models for streams and rivers range from relatively simple analytical models to more sophisticated unsteady flow models. In stream and river systems, water quality gradients generally are greatest or are assumed to be greatest along the flow axis, and one-dimensional (longitudinal) models, which use cross-sectional averaging, are usually appropriate. Although this assumption may be valid for much of a modeled stream system, it can be violated for some localized regions, such as near discharges and downstream of the confluence of two streams. Two-dimensional analytical solutions (e.g. Fischer et al. 1980 and Holley and Jirka 1986) resolve the spread and dilution of effluent plumes. These mixing models also address the question of whether a pollutant has been sufficiently diluted to meet discharge standards. Selection of an appropriate mixing model can be tedious if one is not familiar with the various models and their assumptions. The U.S. Environmental Protection Agency, Athens, GA, is incorporating these models and their protocols into an expert system to facilitate their use. This expert system will lead the user through the proper model selection and use.

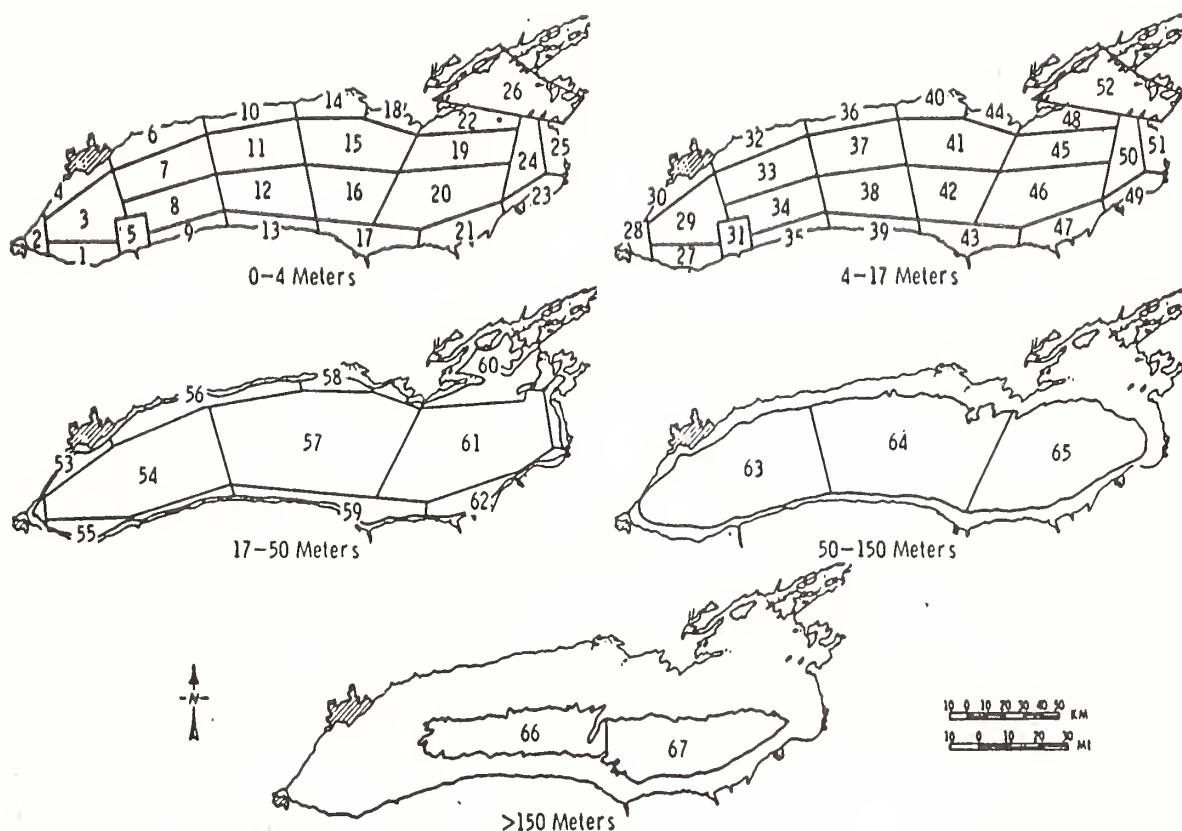


Figure 5.
Lake 3 segmentation (from Thomann et al. 1975).

Herein we distinguish between stream water quality models and stream mixing models. Water quality models predict changes in water quality constituents due to transport, loadings, and reactions. Stream mixing models typically predict the initial mixing, spread and dilution (as discussed above), and sometimes downstream transport of a pollutant loading, but they do not include constituent interactions and reactions. Stream mixing models treat the pollutant as conservative and are therefore not appropriate for farfield stream water quality studies. For the latter, 1-D models are used and often instantaneous mixing of the effluent across the stream is assumed. Although this assumption contradicts reality in localized regions near discharges, it is a practical and meaningful way of addressing most stream water quality issues. A variety of 1-D stream water quality models exist, ranging from steady-state analytical solutions to dynamic numerical models.

Analytical and Numerical Steady-state Models of Stream and River Water Quality

Analytical solutions for 1-D stream water quality models can be derived for steady-state DO and BOD with simple first order decay and sedimentation terms. Gromiec et al. (1983) provided formulations and solutions for a number of these models. Steady-state analytical solutions have the advantages that they can be quickly applied and have minimal data requirements. Their major disadvantages are that they require substantial simplification of stream geometry and that they do not provide time-varying information that may be required to fully address many questions.

Computerization of steady-state, analytical models allows easy simulation of more complex systems, such as stream networks. The USGS Streeter-Phelps model (Bauer et al. 1979) and the U.S. Corps of Engineers STEADY model (Martin 1986) are examples of analytical models that allow a steady-state solution for a stream network. STEADY models temperature, DO, and BOD;

the USGS Streeter-Phelps model computes DO and the components of nitrogenous oxygen demand in addition to CBOD, orthophosphate phosphorus, total and fecal coliform bacteria, and three nondegrading (conservative) substances.

When assumptions that facilitate analytical solutions either become inappropriate or do not allow for enough flexibility, it becomes necessary to resort to numerical water quality models. Numerical water quality models for rivers and streams vary widely in the amount of detail allowed, the number and type of water quality constituents, and whether or not the model allows for time-varying conditions. The following discussion provides an overview of two 1-D, numerical, stream water quality models that are representative of other models of their type.

An example of an intermediate modeling approach between fully dynamic and steady-state models is found in QUAL2E (Brown and Barnwell 1985), a model developed through, and maintained by the U.S. Environmental Protection Agency. QUAL2E is a numerical, 1-D (longitudinal) water quality model which assumes steady flows (steady-state hydraulics) but allows simulation of either steady-state or dynamic water quality (variations). The model allows simulation of 15 water quality constituents: dissolved oxygen, carbonaceous biochemical oxygen demand, temperature, algae as chlorophyll-*a*, organic nitrogen, ammonia nitrogen, nitrite nitrogen, nitrate nitrogen, organic phosphorus, dissolved (inorganic) phosphorus, coliforms, an arbitrary nonconservative constituent, and three arbitrary conservative constituents. QUAL2E has been widely used and is an accepted standard, particularly for waste-load allocation studies of stream systems.

QUAL2E simulates a series of piecewise, nonuniform, steady-flow segments referred to as reaches. Thus, the flows throughout the system are constant with time and uniform within each reach, but the flow and hydraulic characteristics can vary from reach to reach. The model is flexible in allowing the simulation of point and nonpoint loadings, withdrawals, branching tributaries, and in-stream hydraulic structures.

QUAL2E is easier to use than fully dynamic models (time-varying flow and water quality) because of the steady-state hydraulic feature. Hydraulic conditions are determined by any of three methods: 1) using stage-discharge relationships for each reach; 2) solving Manning's equation with prismatic channel geometry information given for each reach; and 3) entering hydraulic information from another external source, such as a hydraulic step calculation (e.g. HEC-2, Hydrologic Engineering Center 1982) or stream gaging information. Time varying flow updates can be used with the model (Hamlin and Nestler 1988) without excessive error if the changes in flow are small and introduced gradually with respect to the system travel time.

Dynamic Models of Stream and River Water Quality

Fully dynamic models are required where transient events are of importance and where significant flow variations occur over periods which are much less than the travel time for the reach of interest. For example, if the travel time for a particular flow is greater than its duration, then only a portion of the reach would be exposed to that flow and its associated quality at a given time. Using steady-state hydraulics, such as in QUAL2E, the flows for all reaches would have to be incremented to the new flow condition instantaneously. In a fully dynamic model, the effects of time-varying flows and quality along the reach are considered. Fully dynamic stream water quality models are time-varying, hydraulic or hydrologic routing models coupled with time-varying constituent transport and transformation models.

A number of fully dynamic, stream water quality models are in existence (see for example, Jobson 1981 and 1987; Hydrologic Engineering Center 1978; and Bedford et al. 1983). A modified version of the Bedford model, referred to as CE-QUAL-RIV1 (Bedford et al. 1982), includes features specifically for regulated streams. CE-QUAL-RIV1 has been applied by the Corps of Engineers to a variety of regulated stream environments, including tailwaters below peaking

hydropower dams, stream regulation (Zimmerman and Dortch 1986), and run-of-the-river navigation pools.

The CE-QUAL-RIV1 modeling package contains two codes, RIV1H for hydraulic routing and RIV1Q for water quality routing. RIV1H, which is similar to Fread's model (1978), solves the nonlinear St. Venant equations using the four-point implicit finite difference method with a Newton-Raphson convergence for non-linearity. The model's formulation allows simulation of dynamically coupled branched river systems with multiple hydraulic control structures, such as weirs and low head dams. Boundary conditions may be provided in terms of flows, stages, or rating curves.

RIV1Q is driven by output from RIV1H or any other flow routing model. RIV1Q uses an explicit finite difference method to solve the constituent mass balance equations. A two-point, fourth-order accurate scheme (Holly and Preissman 1977) is used for the advection term. This means that the model can accurately resolve the transport of sharp water quality gradients with little numerical diffusion. This feature can be important when simulating dynamic flow and loading conditions or when tracking a spill. The model is similar to QUAL2E in that it models temperature, DO, CBOD, and nutrient kinetics. Reaeration takes into account stream reaeration, wind-driven reaeration, and reaeration through control structures.

Inputs and Mixing Zones

Inputs are usually classified as point source (PS) or nonpoint source (NPS). One usually finds higher concentration gradients in the vicinity of a pollutant source than in the receiving water body. The purpose of a mixing zone analysis or model usually is to determine the flow and concentration gradients in the vicinity of point source discharges (Lam et al. 1984).

Mixing zone analysis for point source pollution can have two different objectives: (a) to show sufficient dilution of an effluent near its discharge point so that a specified concentration (effluent WQ standard) is not exceeded beyond specified distances from the outlet or (b) to determine the distance required to mix an effluent nearly uniformly (e.g. $0.9 \bar{C} < C < 1.1 \bar{C}$) with a river cross section or a layer in a stratified reservoir.

A mixing zone model describes the location of the isopleths as a function of river and outlet channel geometry, river flow, and effluent flow conditions. The development of the model must take into consideration the hydrodynamics of the situation. For example, a side channel discharge interacts with a river flow in several ways before the two become fully mixed. Among the flow and mixing processes generally to be considered are (Stefan 1982, 1984; Muellenhoff 1985): a) jet effects due to the momentum of the discharge; b) lateral displacement of river flow by the effluent input; c) downstream advection by the river flow; d) transverse turbulent mixing including secondary flow in the river; e) buoyant spreading caused by the density difference between effluent water and river water--density depends on water temperature and total solids content; f) vertical turbulent mixing by the river due to bed shear; and g) mixing by navigation, structures and similar man-made effects.

To facilitate the analysis it can sometimes be considered that some of the processes occur in sequence (e.g. jet mixing before buoyancy effects). Effluent models are usually subdivided into a NEARFIELD and a FARFIELD (fig. 6). In the nearfield the mixing and dilution are influenced hydrodynamically by effluent conditions. In the farfield, the mixing is passive and is imposed by the receiving water conditions. Farfield models are usually 2-D and use the advection/diffusion equation in either a horizontal or vertical plane (Krishnappan and Lau 1982, 1985). If the effluent and the receiving water differ in density, a density-stratified flow may develop, especially if the receiving water is an impounded river or a lake.

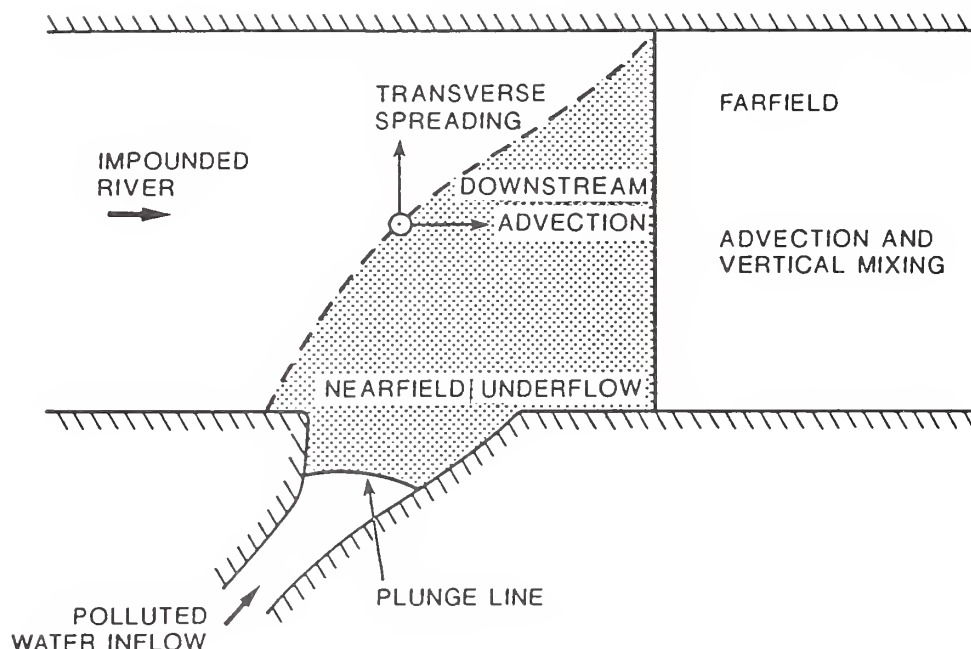


Figure 6.
Nearfield and farfield of a buoyant effluent in an impounded river.

When effluent discharges are from pipes, the nearfield mixing analysis may require the application of jet flow models, and in the case of complex geometries recourse to physical models. Specialized numerical models exist for the analysis of point-source releases, e.g. DISPER or TADPOL (Almquist et al. 1977) for passive mixing in the farfield, and various jet and plume mixing models in uniform or stratified ambients, e.g. EPA's PDS model and Ditmars', 1969 submerged jet models. For discussion of this highly specialized topic, see Fischer et al. (1980) and Holley and Jirka (1986).

SEDIMENT TRANSPORT AND SEDIMENT/WQ INTERACTIONS

Concepts

Sediment is typically associated with agricultural runoff. Sediment not only affects water clarity but can carry chemicals such as nutrients and toxic substances into receiving waters. Therefore, an important aspect of water quality modeling is the capability to simulate sediment transport and sediment/water interactions.

Aquatic sediment transport has two main forms: bed load and suspended load. Although both forms of transport can be important in streams, suspended transport is of primary interest in standing waters. Even when there is no sediment transport by the flow, sediments deposited on the bed of a stream, reservoir or lake, and not in motion can have a strong influence on water quality in the overlying water. Through adsorption, biofilm and other chemical/biochemical transformations, stream or lake sediments can become sinks or sources of materials such as oxygen, toxic materials, or nutrients.

For water quality, suspended sediment and moving or stationary bed sediments are of primary interest, particularly for the finer fractions of materials including silts, clays, organic detritus and live plankton materials. Particles are characterized by size, shape, density, surface area, and

surface physical and chemical properties including electric charges. A review of particle regimes, composition, behavior and interaction with water density was given by Lal (1977).

Processes

Fall Velocities, Settling, Deposition

The fall velocity of particles, and their resistance to resuspension under shear stress, once they are deposited, are most significant for water quality modeling. Fall velocities are functions of size, shape (drag coefficient) and density and can be reasonably well predicted for larger mineral particles (Dietrich 1982, Gibbs et al. 1971). For micron-size particles and particularly for organic particles, the large diversity in sizes, shapes, and density (Lal 1977; Ives 1973) often require indirect determinations of fall velocities from settling traps or mass balances. Settling velocities are used to calculate the movement of sorbed chemical downward through the water column. The deposition velocity can be estimated as the product of the settling velocity and the probability of deposition upon contact with the bed, which may range from 0 for fast, turbulent streams to 1 for stagnant pools.

Resuspension, Scouring, Erosion

Rates of resuspension under bedshear action are difficult to determine. For granular noncohesive materials, the relationship is explosive in nature. Very low or no resuspension occurs until a threshold shear stress is reached. Then resuspension rates increase proportional to some power of the excess shear stress. A power of one has been found in estuarine studies, but powers of four and five have been found for granular river material according to a review by Akiyama and Fukushima (Wang et al. 1986). Rate of resuspension can be balanced by rate of deposition. At that point vertical concentration profiles above the bed show a balance of downward fluxes of sediment by settling and upward fluxes by turbulence as summarized by Vanoni (1975). According to Rouse (see Vanoni 1975), the dimensionless parameter $V_s(\kappa u^*)^{-1}$ determines, for flow over flat bottoms, how uniform vertical sediment distribution will be. It will be uniform within ± 10 percent when $V_s(\kappa u^*)^{-1}$ is less than ~ 0.02 . V_s = particle fall velocity [LT^{-1}], $\kappa = 0.4$ and $u^* =$ bed shear velocity = $\sqrt{\tau_b/\rho}$ [LT^{-1}] with τ_b = bed shear [ML^{-2}] and ρ = water density [ML^{-3}].

Rates of resuspension of noncohesive materials have been specified in numerous alternative forms by Ariathurai (1982), Ariathurai and Krone (1976), and others (see Wang et al. 1986, Mehta 1986). Akiyama and Fukushima (in Wang et al. 1986) specified a dimensionless resuspension rate parameter, E_s , as:

$$E_s = \begin{cases} 3 \times 10^{-12} Z^{10} (1 - 5/Z) & \text{for } 5 < Z < 13.4 \\ 0.3 & \text{for } Z \geq 13.4 \end{cases} \quad [11]$$

where $Z = \frac{u_*}{V_s} R_p$;
 $R_p = (g' D)^{1/2} D / \nu$;
 $g' = g(\rho_s/\rho - 1)$ = reduced acceleration of gravity of submerged particles [LT^{-2}];
 D = particle diameter [L]; and
 ν = kinematic viscosity [L^2T^{-1}].

The resuspension (or scour or erosion) rate depends not only upon the shear stress on the benthic surface and the sediment size, but also on the state of consolidation of the surficial benthic deposits. Site-specific calibration is necessary to refine initial estimates of scour.

Cohesion

Cohesion of particles in the deposited bed increases the resistance to resuspension and is a function of the degree of consolidation. The investigation of this behavior by Krone, Ariathurai,

Partheniades and others has been reviewed by Mehta (1986). Besides bed shear stresses due to gravity or wind-driven flows, perturbations by navigation or organisms (bioturbation) can greatly increase rates of resuspension of cohesive sediments. Effect on resuspension by wind was conceptualized by Rodney and Stefan (1987).

Coagulation and Flocculation

Coagulation is a physical/chemical process by which particles form flocs. Flocs have higher settling velocities, which affects water quality in a very significant way. This effect is used in waste water treatment. Its significance in freshwater bodies has been studied by O'Melia (1980) among others.

Sorption

Suspended sediment, besides being a very important water quality parameter in its own right can also have a very strong relationship with chemicals dissolved in the water through adsorption/desorption. This is an area of very active research (e.g. Golterman et al. 1984, Stumm and Morgan 1981; Karickhoff 1984) and will be addressed in a later section in more detail.

Bottom Boundary Layer

The interaction between particles and water chemistry becomes particularly complex near the bed because of (a) strong velocity gradients in the vertical associated with shear forces, (b) activities of organisms such as biofilms, invertebrates, crustaceans and fish and (c) pore water movement which leaches into and out of the outlying waters. Microcosm models of these systems are necessary to provide the input or withdrawal rates of dissolved substances. Examples are sedimentary oxygen demand (Chen et al. 1984, Gantzer et al. 1988) phosphorus release, and PCB resuspension.

Turbidity Currents

Suspended sediment can increase the density of the water/sediment mixture enough so that density currents can form in "standing" waters when such mixtures are released near the shore or water surface. Particles can be deposited from such currents or eroded from the bed, and as a result, buoyancy flux is not conserved. Turbidity currents can be generated by wave action in shallow areas of lakes or reservoirs, by longshore currents, or simply by inflows; they provide a mechanism by which pollutants attached to sediment can be rapidly transported over long distances from shallow littoral waters to profundal waters. The mechanics of the erosive phase of such currents and 1-D models for their analysis exist (Akiyama and Stefan 1985) and can be incorporated in reservoir WQ models. The depositional phase of these currents is still under investigation.

Model Formulations

In stratified lakes and reservoirs of moderate size, advection in the horizontal direction is rapid, relative to vertical mixing, and hence only vertical gradients in suspended sediment concentration are simulated. One-dimensionality is often an acceptable assumption for smaller waterbodies (<20 km long). A relationship among suspended sediment concentration profiles, vertical turbulence, rate of deposition, and resuspension is

$$A \frac{\partial(C)}{\partial t} + \frac{\partial(V_s A C)}{\partial z} = V_s C \frac{\partial A}{\partial z} + \frac{\partial}{\partial z} \left(A K_z \frac{\partial C}{\partial z} \right) - R \frac{\partial A}{\partial z} \quad [12]$$

where C = suspended sediment concentration; and
 V_s = fall velocity of suspended sediment in quiescent water.

The first term in this equation represents the change in sediment content with time, the second term is the rate of transfer by settling from one layer to another, the third term is the rate of

deposition on the sloping lake bed, the fourth term is the vertical turbulent mixing rate, and the last term is the resuspension. Vertical advection can be added to this equation.

There exist sediment transport models for specific purposes e.g. modeling of alluvial channels (Dawdy and Vanoni 1986), reservoir sedimentation (Hydrologic Engineering Center 1977) estuarine water movement and sediment transport (King 1982), or simple lake turbidity (Stefan et al. RESQUAL II, 1982). Most of these models can be found referenced in recent proceedings of conferences dealing with river sedimentation (Wang et al. 1986), coastal engineering (Mehta 1986), reservoirs (Stefan 1981; Thomas et al. 1985) and lakes (Lerman 1978). Many of these models are concerned mainly with the quantity of sediment transport, locations of erosional or depositional areas, channel modification etc. Models dealing with suspended particle transport including inorganic and organic (detritus and phytoplankton) particles and their interaction with water quality have been developed mostly for applications in eutrophication control discussed in one of the next chapters.

The following are examples of 1-, 2-, and 3-D sediment transport models.

One-dimensional models.

HEC-6 (Hydrologic Engineering Center, 1977) computes both flow and transport. It is designed to analyze scour and deposition in rivers and reservoirs. HEC-6 and similar models are used when the flow is unidirectional and constrained to follow well-defined channels. It calculates transport of sands, silts, and clays and can handle bed load and suspended load transport. A 1-D turbidity model is the RESQUAL II model (Stefan et al. 1982). It computes the unsteady, vertical distribution of suspended sediment and uses it to determine light penetration for primary productivity. The attenuation coefficient η is calculated as the cumulative effect of the water, the suspended inorganic sediment concentration (SS), and the chlorophyll-*a* concentration (Chl*a*).

$$\eta = a + bSS + c \text{ Chl}a \quad [13]$$

Two-Dimensional Models

Two-dimensional models include those that are integrated over depth (horizontal models) and those that are integrated over width (vertical models).

Horizontal two-dimensional modeling of sediment transport is performed by STUDH, which is part of the TABS-2 modeling system (Thomas and McAnally 1985). STUDH is a finite element model designed for situations where the flow and transport can be satisfactorily described by depth-integrated equations. STUDH computes the bedload or suspended load transport of silts or clays. It obtains flows either by specification or from the TABS-2 flow model, RMA-2V. It calculates transport due either to currents alone or to currents plus short-period waves (nonbreaking). The program allows for wetting and drying of cells and consolidation of fine sediments with overburden and time.

Laterally-averaged models are applicable in studies of relatively deep, narrow water bodies. Work on models of this type has been more limited than on the depth-averaged models. However, work performed during the past few years has produced a useful model, LAEMSED. LAEMSED was produced (Johnson et al. 1987) by adding sediment transport capability to the basic hydrodynamic/transport model LARM2 (Edinger and Buchak 1983) on which CE-QUAL-W2 is also based. A layered bed model allows for the exchange of material between the water column and the bed, but only suspended sediment transport is simulated. This model has been used to investigate the effect of navigation channel deepening on salinity intrusion and sediment transport (Johnson et al. 1987).

Three-Dimensional Models

Two sets of three-dimensional models are in use by the Waterways Experiment Station for suspended sediment transport. They are the RMA series and CELC3D. Both models have a free surface, are time dependent, and allow for stratification and complex geometry.

RMA Series. The RMA series of programs model flow and transport in three dimensions using a finite element method. Program RMA-8 (King 1982) computes water levels and currents for constant density flows. RMA-10 (King 1982) computes water levels, currents, and salinity/temperature transport for flows with density gradients. SEDIMENT 8 (Ariathurai 1982) computes transport for sands, silts, or clays and contains information from Ariathurai and Krone (1976). The models permit parts of the computational mesh to be two-dimensional while employing the full three dimensions in other areas, thus ensuring economical operation.

CELC3D. The 3-D finite difference model of Coastal, Estuarine, and Lake processes, CELC3D (Sheng 1983), simulates hydrodynamics and transport for temperature, salinity, and sediment. Special features include (a) a "mode-splitting" procedure which allows efficient computation of the vertical flow structures (internal mode); (b) an alternating direction implicit (ADI) scheme for the computation of the vertically-integrated variables (external mode); (c) an implicit scheme for the vertical diffusion terms; (d) a vertically and horizontally stretched coordinate system; and (e) a turbulence parameterization. CELC3D provides for the resuspension, transport, and deposition of sediments where sediment particle dynamics are modeled by a consideration of particle groups and coagulation processes. Detailed dynamics within a turbulent boundary layer, under pure wave or wave-current interaction, are evaluated by means of a turbulence submodel.

Other 3-D models of estuaries and coastal seas were developed by Leendertse (1970) and Leendertse and Liu (1975) and Onishi and Trent (1982).

MODELS ADDRESSING ORGANIC WASTES AND NUTRIENTS

Concepts

Water quality problems created by organic waste and nutrients include depletion of dissolved oxygen and stimulation of nuisance aquatic growth. In addition, high levels of nitrate or ammonia can be harmful to aquatic life.

Organic waste is generated by farm operations, and may be carried to ponds and streams by runoff. Nutrients such as nitrogen and phosphorus are applied to fields as fertilizer, and can reach surface waters by runoff and leaching. Nitrogen is soluble and is easily mobilized by runoff or leachate water. Phosphorus is strongly bound to soil, but may be carried by erosion. The organic matter and nutrients contained in agricultural runoff can play an important role in the trophic state and water quality of receiving waters. This section is a brief overview of the processes for modeling these constituents (referred to as conventional pollutants) and their interactions. For more detailed information, see Bowie et al. (1985); Orlob (1983); Chapra and Reckhow (1983); and Thomann and Mueller (1987). The focus of models of conventional pollutants can be dissolved oxygen (DO) and biochemical oxygen demand (BOD) as a general measure of the health of the system, or it can be primary productivity when eutrophication is the major concern. These models usually include temperature, major nutrients, other chemical characteristics, detritus, bacteria, and primary producers. Water quality models for surface waters may include higher trophic levels (i.e. zooplankton and fish) because of their effect on other more important variables, such as phytoplankton, BOD and DO. Zooplankton and fish also provide a means of controlling lower trophic levels, which can affect nutrients and DO (biomanipulation). Because the source of agricultural organic waste and nutrients is driven by the hydrologic cycle, the most appropriate

modeling approaches are dynamic. However, for leaching or irrigation situations steady state or quasidynamic models may be adequate.

Fate Processes

Upon entry to the surface water body, particulate organic waste and nutrients usually settle. High flow events, however, may lead to scouring of previously deposited material. Organic matter is oxidized, drawing upon the dissolved oxygen supply, which is replenished by reaeration. Organic nitrogen is mineralized to ammonia, which reaches ionic equilibrium with ammonium. Nitrification further draws upon the dissolved oxygen supply, converting ammonia to nitrite and then nitrate. Nitrate may be converted back to ammonia or to nitrogen gas through denitrification in low DO regions of the water or sediment. Ammonia and nitrate may be taken up by phytoplankton and aquatic plants and incorporated into the food chain, eventually returning to the water as organic nitrogen.

Organic phosphorus is mineralized to orthophosphate, which comes to sorptive equilibrium with suspended or benthic sediment. Particulate-sorbed phosphate settles; dissolved phosphate is rapidly taken up by phytoplankton and aquatic plants and incorporated into the food chain, eventually returning to the water as organic phosphorus.

Organic material deposited as benthic sediment is oxidized in the upper aerobic layer, and reduced in the lower anaerobic layers. Upward fluxes of ammonia and reduced organic species are produced, the latter contributing to sediment oxygen demand. Particulate phosphorus may be resolubilized and reenter the water. In some aquatic environments, net sedimentation buries a large fraction of the nutrients and organic matter deposited to the bed.

Although many of these interacting fate pathways are well known and included in most recent conventional water quality models, accurate simulations remain difficult. Extensive site-specific data collection is required to characterize both the sources and the rates under a range of expected conditions. Many of the rates are biologically mediated, with descriptive constants and parameters that vary both with environmental conditions and predominant species. The major pathways and cycles will be briefly discussed from the model developer's perspective.

Phytoplankton Kinetics

Phytoplankton kinetics assume a central role in eutrophication affecting the nitrogen and phosphorus cycles, the dissolved oxygen balance, and food chain response. The reaction term for phytoplankton is expressed as the difference between the growth rate and the death and settling rates in a volume element. The growth rate of phytoplankton is a complicated function of the species present and their differing reactions to solar radiation, temperature, and the balance between nutrient availability and phytoplankton requirements. Available information does not allow specification of growth kinetics for individual species in a natural environment. Hence, models either simulate the phytoplankton community as a whole, or as classes such as greens, diatoms, blue-greens, and dinoflagellates.

The growth rate G is usually formulated as the product of the maximum 20°C growth rate (under optimum light and nutrient conditions) with a temperature adjustment factor, a light adjustment factor, and a nutrient limitation factor

$$G = G_{\max} X_T X_L X_N \quad [14]$$

Temperature is an important water quality variable because of its effects on transformation and reaction rates and aquatic life. Temperatures are calculated as described in the section on 1-D temperature-stratified reservoir models. The temperature adjustment factor is usually given as

$$X_T = \theta^{T-20^\circ} \quad [15]$$

where θ is a species-specific coefficient.

Light attenuation functions, X_L , generally follow the analysis by Steele (1965), accounting for the effects of supersaturating light intensities and light attenuation through the water column, and lead to

$$X_L = \frac{2.718}{\eta d} \left[\exp \left\{ - \frac{I_0}{I_s} \exp(-K_e D) \right\} - \exp \left\{ - \frac{I_0}{I_s} \right\} \right] \quad [16]$$

where d = depth [m];
 η = light extinction coefficient (including self shading) [m];
 I_0 = incident light intensity just below the surface [ly/day]; and
 I_s = saturating light intensity of phytoplankton [ly/day].

The expression is either integrated over the day or multiplied by the daylight fraction. I_s is generally used as a calibration parameter. Smith (1980) developed a framework for calculating I_s based upon the maximum growth rate, the quantum yield of chlorophyll, the extinction coefficient per unit of chlorophyll, and the ratio of carbon to chlorophyll in the phytoplankton. This framework allows for adaptation by changing the carbon to chlorophyll ratio. Recent developments in phytoplankton kinetics models use photosynthetically active radiation (PAR) [$\mu\text{Em}^{-2}\text{day}^{-1}$] instead of total energy, I_s [la day^{-1}]. They also apply Haldane kinetics in place of Steele's equation (see Megard et al. 1984).

The nutrient limitation factor is based on the assumption that phytoplankton follow Monod kinetics with respect to the important nutrients. Generally, the minimum function for inorganic nitrogen and phosphorus is used

$$X_N = \text{Min} \left\{ \frac{C_{IN}}{K_{MN} + C_{IN}}, \frac{C_{IP}}{K_{MP} + C_{IP}} \right\} \quad [17]$$

where C_{IN} = inorganic nitrogen [$\mu\text{g}/\ell$];
 C_{IP} = inorganic [$\mu\text{g}/\ell$];
 K_{MN} = Michaelis half-saturation constant for nitrogen [$\mu\text{g}/\ell$]; and
 K_{MP} = Michaelis half-saturation constant for phosphorus [$\mu\text{g}/\ell$].

Occasionally, X_N is expressed as the product of the nitrogen and phosphorus terms.

Phytoplankton "death" rates are conventionally expressed as the sum of the endogenous respiration rate, the death rate, and the grazing rate. The first two are generally modeled as first order temperature corrected rates. Grazing may be expressed as first order, or second order if the herbivorous zooplankton population is specified or simulated. To capture the phytoplankton population dynamics properly, zooplankton may have to be simulated. If average phytoplankton levels are adequate, then the first order approach is acceptable.

Phytoplankton kinetics affect the nitrogen, phosphorus, and carbon cycles primarily through uptake and secondarily through death. Proper specification of average stoichiometry is necessary to accurately model these interactions. The ratios of phytoplankton carbon to phytoplankton nitrogen, phosphorus, and chlorophyll- a vary among species and in time. Few applied modeling frameworks account for the dynamics of stoichiometry. The user is forced to specify average values or those characteristic of stressed systems.

The Phosphorus Cycle

Organic phosphorus in the water is present in various particulate and dissolved forms that mineralize and settle at different rates. Some models lump all organic phosphorus into a single state variable; while others divide organic phosphorus into two-, three-, or four-state variables that differ in settling and mineralization rates. Mineralization or bacterial decomposition is generally modeled as a first order temperature-corrected reaction, although second order and saturating rates based upon phytoplankton biomass have been used.

Dissolved inorganic phosphorus sorbs to suspended particulate matter in the water column, coming to an equilibrium expressed either with a partition coefficient or as a calibrated fraction dissolved

$$f_{DIP} = \frac{1}{1 + K_{PIP}SS} \quad [18]$$

where f_{DIP} = fraction inorganic phosphorus dissolved;
 SS = suspended sediment concentration [kg/l]; and
 K_{PIP} = partition coefficient [l/kg].

Subsequent settling of the solids and sorbed phosphorus can provide a significant loss mechanism of phosphorus from the water column to the benthos. Process-based functions that accurately calculate the phosphorus partition coefficient would improve prediction of this important variable significantly. Phytoplankton take up phosphorus at the dissolved inorganic phosphorus stoichiometrically modified growth rate. While there is evidence for "luxury storage" of inorganic phosphorus in phytoplankton, most models assume only one internal pool of phosphorus as biomass. Grazing causes transfer of phytoplankton phosphorus up the food chain. Upon respiration and death, biomass phosphorus is recycled to the various forms of organic and inorganic phosphorus at user-specified ratios.

The Nitrogen Cycle

Organic nitrogen in the water is present as various particulate and dissolved forms that mineralize and settle at different rates. As for organic phosphorus, some models lump all organic nitrogen into a single state variable, whereas others divide organic nitrogen into two, three, or four state variables. Mineralization to ammonia can be represented as first order, or include second order or saturating dependence on phytoplankton biomass.

Ammonia nitrogen in the presence of nitrifying bacteria and oxygen is converted to nitrite then nitrate nitrogen. Nitrification in natural water is complex, depending upon dissolved oxygen, pH, total inorganic carbon, alkalinity, Nitrosomonas and Nitrobacter bacteria, and flow conditions. Most models represent the reaction with a first-order, temperature-corrected rate constant. Some allow spatial variations calibrated by the user, or empirical DO limitation terms. Obviously, a process-based predictive function for this rate would be quite valuable.

Denitrification is the reduction of nitrate to ammonia and nitrogen gas. Primarily a benthic reaction, it is included in some models as a loss rate of nitrate. It is modeled as a first order reaction, sometimes multiplied by a modified Michaelis-Menten term to suppress the reaction in the presence of a small amount of oxygen.

Both ammonia and nitrate are taken up by phytoplankton at the stoichiometrically modified growth rate. Some models include a preference function that calculates mostly ammonia uptake when its concentration is high enough. Grazing causes transfer of phytoplankton nitrogen up the food chain. Upon respiration and death, biomass nitrogen is recycled to the various forms of organic nitrogen and ammonia at user specified ratios.

The Carbon-Dissolved Oxygen Balance

Organic carbon is present in water in various particulate and dissolved forms that oxidize and settle at different rates. Some models lump all organic carbon into a single state variable expressed in units of oxygen--carbonaceous biochemical oxygen demand, CBOD. Other models represent various fractions of organic carbon, with their separate oxidation and settling rates. Oxidation is generally modeled a first-order temperature-corrected rate. Some allow spatial variations calibrated by the user.

Traditional models of organic waste do not compute inorganic carbon and the associated variables of pH and alkalinity. This carbonate system could be important for simulating the effects of acidic wastes on un-ionized ammonia concentrations or potential carbon dioxide limitation in low alkalinity, high nutrient waters. Models that include the carbonate system calculate total inorganic carbon as the sum of bicarbonate, carbonate, and carbon dioxide. These species are in equilibrium controlled by the equilibrium constants of the dissociation reactions and the pH of the water. Carbon dioxide (and thus total inorganic carbon) is produced by respiration, consumed by algal growth, and replenished by atmospheric exchange. Carbonate alkalinity is the sum of bicarbonate concentration, two times the carbonate concentration, and the hydroxide concentration minus the hydrogen ion concentration. Addition of acids and nitrification lower the pH and reduce alkalinity. Nitrate uptake by phytoplankton produces hydroxide and increases alkalinity.

Dissolved oxygen is depleted by oxidation of organic carbon, nitrification, and respiration. Benthic reactions depleting oxygen are usually modeled as a spatially variable flux of sediment oxygen demand. Respiration effects may be combined for simplicity or separated into components such as respiration by bacteria, plankton, macrophytes, fish, etc. The respiration of decomposers that utilize organic matter is referred to as decomposition. Oxygen is used during some chemical transformations, such as nitrification and the oxidation of reduced substances (e.g. sulfide, methane, reduced iron, and reduced manganese). Biochemical oxygen demand (BOD) is a measure of the oxidizable matter due to biochemical processes. The problem with BOD is that it combines the effects of several oxygen consuming processes into one variable; this approach may be too simple for modeling some systems. The more realistic approach is to separate oxygen demands into various components, such as biodegradable organic (carbonaceous) demands, nitrogenous demands, and oxidation of other substances (e.g. reduced metals and sulfide). Biodegradable organic demands may be due to dissolved and particulate matter in the water column and bottom sediments. Some models separate water column organic matter into particulate and dissolved forms, referred to as POM and DOM. Because some forms of organic matter decay faster than others, organic matter may be further divided into those that decay fast (labile) and those that decay slower (refractory). As labile organic matter decomposes, a portion is transferred to the refractory state. A similar approach can be used for organic sediments. Sources of organic matter include external waste loads and excretion, and mortality of living substances.

Dissolved oxygen is replenished by phytoplankton growth (photosynthesis) and by reaeration. Many reaeration formulas exist for streams and rivers. Those based solely on velocity and depth include O'Connor-Dobbins (for slow, deep rivers), Churchill (for moderately deep, fast streams) and Ownes et al. (for shallow streams). (See Thomann and Mueller 1987). The Tsvoglou method calculates reaeration in rivers and streams from the slope and travel time. Relationships which include the effects of bed roughness, secondary flow and wind are under development. Numerous relationships exist for wind-induced reaeration in lakes and reservoirs. There remains a need for critical review and assimilation of all the formulas. Reaeration at hydraulic structures can be very significant.

Benthic-Water Interactions

The decomposition of organic material in benthic sediment can significantly affect the concentrations of oxygen and nutrients in the overlying waters. Areal fluxes from the sediment

due to diagenetic reactions can be substantial nutrient sources or oxygen sinks. Anoxia may dramatically increase nutrient fluxes.

Most traditional models described these benthic fluxes as spatially variable source and sink terms. Some recent models have included benthic compartments where state variables are simulated. Particulate nitrogen, phosphorus, and carbon are added to the bed by settling, and lost by scour or sedimentation (burial). Dissolved species of nitrogen, phosphorus, carbon, and oxygen exchange with overlying water by pore water diffusion. Benthic oxidation rates are generally assumed first-order, with low rate constants producing ammonia and consuming organic carbon and oxygen equivalents (functionally, reduced organic species that are oxidized at the water interface). Recently, efforts have been made to simulate the diagenetic reactions and resulting fluxes more realistically (DiToro 1986). These efforts hold great promise for more accurate and predictive modeling of organic and nutrient wastes.

Simulation Models

Numerous simulation models of organic waste and nutrients have been developed and applied to various water bodies. Of these, only a few have been maintained for general application. To be useful for general agricultural nutrient and organic waste simulations, a model should allow for unsteady transport and loading, phytoplankton kinetics, nitrogen and phosphorus cycles, and carbon-dissolved oxygen balances. Furthermore, written documentation and a users manual must be available with the software.

Five modeling frameworks meet these criteria: WASP4-(EUTRO4), CE-QUAL-R1, CE-QUAL-W2, CE-QUAL-RIV1, and HSPF. QUAL2E may be useful for steady loading situations. Such models as DEM, EXPLORE, RECEIVII, WRECEV, MINLAKE, and AUTO-QD meet these criteria but are not actively maintained and supported by a central, public distribution center. Different versions of these and others may be maintained by consultants and local government agencies, and be useful for those water bodies where setup and calibration have already been done.

Stream Quality Model QUAL2E (Brown and Barnwell 1987) is a steady-state model for conventional pollutants in one-dimensional streams and well-mixed lakes. The conventional pollutants include conservative substances, temperature, bacteria, biochemical oxygen demand, dissolved oxygen, nitrogen, phosphorus, and algae. QUAL2E is widely used for waste load allocations and discharge permit determinations in the United States and other countries. WASP is designed to permit easy substitution of user-written routines into the program structure. Problems that have been studied using WASP include biochemical oxygen demand, dissolved oxygen dynamics, nutrients and eutrophication, bacterial contamination, and toxic chemical movement.

Eutrophication WASP (EUTRO4; Ambrose et al. 1987) combines a kinetic structure adapted from the Potomac Eutrophication Model with the WASP transport structure. EUTRO4 predicts dissolved oxygen, carbonaceous biochemical oxygen demand, phytoplankton, carbon, and chlorophyll-*a*, ammonia, nitrate, organic nitrogen, and orthophosphate in the bed and overlying waters.

WASP4 is linked to DYNHYD4 (Ambrose et al. 1987) a simple link-node hydrodynamic model capable of handling variable tidal cycles, wind, and unsteady inflows. It produces an output file that can be linked with WASP4 to supply the flows and volumes to the water quality model.

Hydrological Simulation Program - FORTRAN (HSPF) (Johanson et al. 1984; Donigian et al. 1984) is a comprehensive package for simulation of watershed hydrology and water quality for both conventional and toxic organic pollutants. HSPF incorporates the watershed-scale ARM

(Agricultural Runoff Model) and NPS (Non-Point Source) models into a basin-scale analysis framework that includes pollutant transport and transformation in stream channels.

The model uses information such as the time history of rainfall, temperature, and solar radiation; land surface characteristics such as land use patterns and soil properties; and land management practices to simulate the processes that occur in a watershed. The result of this simulation is a time history of the quantity and quality of runoff from an urban or agricultural watershed. Flow rate, sediment load, and nutrient and pesticide concentrations are predicted. The program takes these results, along with information about the stream network and point source discharges, and simulates instream processes to produce a time history of water quantity and quality at any point in a watershed--the inflow to a lake, for example. HSPF includes an internal data base management system to process the large amounts of simulation input and output. The models CE-QUAL-R1, CE-QUAL-W2, and CE-QUAL-RIV1 were discussed in previous sections.

SYNTHETIC ORGANIC CHEMICALS

Fate Processes

Ionization

Ionization is the dissociation of a chemical into multiple charged species. Consider a weak acid AH_3 or base BH_3



These reactions are rapid. At equilibrium, the distribution of chemicals between the un-ionized and the ionized species is controlled by the pH of the water and the ionization constants.

Stronger acids and bases may undergo further ionization, controlled by ionization constants K_{a2} , K_{a3} , K_{b2} , and K_{b3} . Ionization can be important because of the different toxicological and chemical properties of the un-ionized and ionized species.

Sorption

Sorption is the bonding of dissolved chemicals onto solid phases S_i , such as benthic and suspended sediment, biological material, and sometimes dissolved or colloidal organic material



These reactions are usually fast relative to other environmental processes, and equilibrium may be assumed. For environmentally relevant concentrations (less than $10^{-5}M$ or one-half water solubility), equilibrium sorption is linear with dissolved chemical concentration (Karickhoff 1984) or

$$C_i = K_{pi}C_d \quad [22]$$

where C_i = chemical concentration in phase i [mg/kg];
 C_d = dissolved chemical concentration [mg/l]; and
 K_{pi} = sorption partition coefficient for phase i [l/kg].

At equilibrium, then, distribution among the phases is controlled by the partition coefficients K_{pi} . The total mass of chemical in each phase is controlled by K_{pi} and the amount of solid phase present.

Values for the partition coefficients can be obtained from laboratory experiments. For organic chemicals, lab studies have shown that the partition coefficient is related to the hydrophobicity of the chemical and the organic matter content of the sediment. Normalization of the partition coefficient by the organic-carbon content of the sediment has been shown to yield a coefficient, K_{OC} , that is relatively independent of other sediment characteristics or geographic origin. Correlation of K_{OC} with the water solubility of the chemical or the octanol/water partition coefficient of the chemical has yielded successful predictive tools for incorporating the hydrophobicity of the chemical in an estimate of its partitioning. These correlations do poorly for chemicals with very low or very high hydrophobicity, however, because of deviations from hydrophobic adsorption. Chemicals containing polar functional groups and low octanol/water partition coefficients tend to exhibit hydrophilic contributions to adsorption, whereas large nonpolar molecules with high octanol/water partition coefficients generally require long time periods to reach equilibrium resulting in low estimates of K_{OC} when sorption is measured over short time frames. The latter effect is particularly significant because it suggests that the assumption of instantaneous equilibrium used by the toxic chemical models may not be valid for those chemicals for which adsorption is the most important process.

In addition to the assumption of instantaneous equilibrium, implicit in the use of equation 22 is the assumption of reversibility. Laboratory data for very hydrophobic chemicals suggest, however, that a hysteresis exists, with desorption being much slower than adsorption. Karickhoff (1981, 1984) suggests that this effect may be the result of intraparticle kinetics in which the chemical is slowly incorporated into components of the sorbent. This phenomenon is not well understood. A quantitative modeling framework to characterize it was proposed by DiToro (1985).

Sorption can be important in controlling both the environmental fate and the toxicity of chemicals. Sorption may cause the chemical to accumulate in bed sediments or bioconcentrate in fish. Sorption may retard such reactions as volatilization and base hydrolysis, or enhance other reactions including photolysis and acid-catalyzed hydrolysis.

Settling, Deposition, and Scour

Suspended particles carrying sorbed chemicals can settle through the water column and deposit on the underlying bed. Benthic particles carrying sorbed chemicals can scour and become suspended in the water column. Mass fluxes for settling, deposition, and resuspension are controlled by the settling, deposition, and scour velocities, and the suspended and benthic sediment concentrations.

Loss Kinetics

Chemical concentrations and resulting toxic effects often decline downstream due to physical and chemical reactions. For constant environmental conditions, the overall chemical loss rate is often approximated as a first-order reaction

$$m_k = -K_T CV \quad [23]$$

where K_T = observed loss coefficient [days^{-1}];
 C = total chemical concentration [g/m^3]; and
 V = volume of water plus sediment [m^3].

K_T represents a single set of environmental conditions only. Changes in temperature, velocity, depth, sunlight, wind, sediment concentration, or pH can affect the total loss rate in unknown ways.

A method to complement field survey data is the chemical process approach. This approach combines laboratory-measured chemical constants with field-measured environmental properties to estimate site-specific rate coefficients, $K_i(x,t)$, for several loss processes "i"

$$K_i(x,t) = K_i E_i(x,t) \quad [24]$$

where K_i = a laboratory measured second-order rate constant and
 $E_i(x,t)$ = the intensity of the relevant environment parameter.

If more than one loss process is active for a chemical in an environment, the overall loss coefficient can be estimated by summing the individual rate constants. Combining the chemical process approach with the field survey approach should increase the reliability of modeling estimates, allowing extrapolation to a much wider range of environmental conditions.

The loss processes considered in most chemical fate models include volatilization, hydrolysis, photolysis, and bacterial degradation. Chemical oxidation and reduction are sometimes included as well.

Volatilization. Volatilization is the flux of a chemical across the air-water interface. Its rate is proportional to the gradient between the dissolved concentration and that of the overlying atmosphere. For most chemicals, the partial pressure in the atmosphere is negligible and the equation reduces to a first-order form with the removal rate coefficient, K_v , expressed as

$$K_v = -k_v f_d d^{-1} \quad [25]$$

where d = the average water depth in [L],
 f_d = the fraction of the chemical concentration that is dissolved, and
 k_v = the conductivity of the chemical in $[LT^{-1}]$.

The conductivity is influenced by both chemical properties (molecular weight, Henry's Law constant) and environmental conditions at the air-water interface (turbulence-controlled by wind speed, current velocity, and water depth). Toxic chemical models either require the user to input a value for k_v or internally compute a value using the two-film theory first proposed by Lewis and Whitman (1924). This theory assumes that the rate of transfer is controlled by diffusion through laminar layers in the air and water at the interface in which the concentration gradients are localized.

The liquid and gas transfer coefficients are dependent on turbulence at the interface, on temperature, and on properties of the chemical such as diffusivity. Empirical correlations have been developed relating transfer coefficients either directly to physical parameters such as wind velocity and the density and viscosity of the water (MacKay and Yeun 1983; Southworth et al. 1979a), plus the molecular weight and diffusivity of the chemical or to the field-measured transfer coefficients of oxygen and water vapor (Liss et al. 1974). O'Conner (1983) has presented a theoretical development of the liquid transfer coefficient applicable to a wide range of hydrodynamic conditions, but application requires estimates of several coefficients and wind data that are not easily obtained.

Hydrolysis. Hydrolysis is a reaction in which cleavage of a molecular bond of the chemical breaks and forms a new bond with either the hydrogen or the hydroxyl component of a water molecule. Hydrolytic reactions are usually catalyzed by acid and/or base, and the overriding factor affecting hydrolysis rates at a given temperature is generally hydrogen or hydroxide concentration (Wolfe 1980). The overall hydrolysis rate constant in most toxic chemical models is calculated by

$$K_H = \sum (k_{HAi}[H^+] + k_{HNi} + k_{HBi}[OH^-]) \quad [26]$$

where k_{HAi} = acid hydrolysis rate constant for phase i [L mole⁻¹],
 k_{HNi} = neutral hydrolysis rate constant for phase i [T⁻¹],
 k_{HBi} = alkaline hydrolysis rate constant for phase i [L mole⁻¹],
 $[H^+]$ = hydrogen ion concentration [moles L⁻¹], and
 $[OH^-]$ = hydroxide ion concentration [mole L⁻¹].

The models do not compute hydrogen or hydroxide ion concentrations. Instead these are input to the models assuming that their concentrations are unaffected by the hydrolysis reaction because of the low concentration of the toxic chemical present and reacting.

Photodegradation. Photodegradation (photolysis) is the transformation or degradation of a compound that results directly from the absorption of light energy. It is a function of the quantity and wavelength distribution of incident light, the light absorption characteristics of the compound, and the efficiency at which absorbed light produces a chemical reaction. Photolysis is classified into two types that are defined by the mechanism of energy absorption. Direct photolysis is the result of direct absorption of photons by the toxic chemical molecule. Indirect or sensitized photolysis is the result of energy transfer to the toxic chemical from some other molecule that has absorbed the radiation.

A quantitative framework that permits the prediction of photolysis directly from the incident light and the characteristics of the chemical (Zepp and Cline 1978) has been incorporated in several of the toxic chemical modeling frameworks. Use of this framework in natural water systems is complicated by the lack of a satisfactory model of UV-light penetration that incorporates the effects of both dissolved organics and particulate material in the water. A comprehensive framework for photolysis also must include sensitized photolysis. Unfortunately, the spectrum of compounds, particularly dissolved organics, involved in photochemical reactions is not known (Miller 1983). In addition, valid frameworks to predict free radical reactions have not been developed and the importance of these reactions remains undetermined (Zepp 1980).

A less rigorous method for predicting a photolysis rate coefficient K_p involves extrapolations of observed rates from one environmental condition to another

$$K_p = K_{PG} L \sum_i \phi P_i f_i \quad [27]$$

where K_{PG} = the observed rate coefficient [T⁻¹] for a reference light intensity,
 L = the fraction of the reference light intensity averaged through the water column,
 ϕP_i = the relative yield for the chemical in phase i, and
 f_i = fraction of the total chemical concentration in phase i.

The reference light fraction, L , accounts for depth, light extinction, cloud cover, latitude changes, and surface light variability.

Biodegradation. Biodegradation encompasses the broad and complex processes of enzymatic attack by organisms on organic chemicals. Bacteria, and to a lesser extent fungi, are the mediators of biological degradation in surface water systems. Dehalogenation, dealkylation, hydrolysis, oxidation, reduction, ring cleavage, and condensation reactions are all known to occur either metabolically or via co-metabolism. Co-metabolism refers to degradation of chemicals by microorganisms that cannot use the chemical as a substrate for growth. Biodegradation is generally assumed to follow Michealis-Menten enzyme kinetics. Values for the half saturation constant K_m and the maximum rate of degradation are not easily measured. Toxic chemical models generally assume the chemical concentration is much less than the half saturation constant and simplify the Michaelis-Menten equation to

$$K_B = -B_{\max} K_m^{-1} B = -k_B B$$

[28]

where K_B = second order rate coefficient (mL/cells-day).

The bacterial activity, B , in cells/mL, is fundamentally the concentration of the enzyme reacting with the toxic chemical. Enzyme concentration cannot be measured in the field, however, and the environmental and ecological effects on its activity are difficult to estimate (Lewis et al. 1984).

The growth kinetics of the bacterial population degrading a toxic chemical are not well understood. The presence of competing substrates and of other bacteria, the toxicity of the chemical to the degrading bacteria, and the possibilities of adaptation to the chemical or co-metabolism make quantification of changes in the population difficult. As a result, toxic chemical models assume a constant biological activity rather than modeling the bacteria directly. Often, measured first-order biodegradation rate constants from other aquatic systems are used directly.

Simulation Models

Numerous simulation models have been developed for toxic chemicals in surface water systems. Of these, only a handful have been developed for general application. To be useful for general agricultural chemical simulations, a model must include benthic and water column compartments, unsteady transport and loading, partitioning and transformation reactions. Furthermore, written documentation and a user's manual must be available along with the software.

Seven modeling frameworks described here meet these criteria: EXAMS (Burns et al. 1982, 1985), a quasidynamic model for organics; WASP (DiToro et al. 1983; Ambrose 1983, 1986a; Ambrose et al. 1987; Connolly et al. 1984a and 1984b) and HSPF (Johanson et al. 1984), dynamic compartment models for organics and metals; SERATRA (Onishi et al. 1982), FETRA and TODAM, one- and two-dimensional dynamic models for organics and metals; and UTM-TOK (Browman et al. 1983), a dynamic multimedia model for organics and metals. These frameworks differ mainly in the degree of specificity incorporated in the transport, transfer and reaction processes, the allowable spatial and temporal resolution of the problem, and the manner in which sediment is defined.

Exposure Analysis Modeling System (EXAMS-II), is both a steady-state and a quasi-dynamic model designed for rapid evaluation of the behavior of synthetic organic chemicals in aquatic ecosystems, including lakes, rivers, and estuaries. EXAMS-II is an interactive program that allows the user to specify and store the properties of chemicals and ecosystems, modify the characteristics of either via simple English-like commands, and conduct rapid, efficient evaluations of the probable fate of chemicals. EXAMS-II simulates a toxic chemical and its transformation products using second-order kinetics for all significant organic chemical reactions. EXAMS-II does not simulate the solids with which the chemical interacts. The concentration of solids must be user-specified for each compartment. The model accounts for sorbed chemical transport based on solids concentrations and specified transport fields. Benthic exchange includes pore water advection, pore water diffusion, and solids mixing. The latter describes a net steady-state exchange associated with solids that is proportional to pore water diffusion. EXAMS is supported by EPA's Center for Exposure Assessment Modeling, Athens, GA.

Water Quality Analysis Simulation Program (WASP4) (Ambrose et al. 1987) is a generalized modeling framework for contaminant fate in surface waters including lakes, rivers, and estuaries. Based on the flexible compartment modeling approach, WASP4 can be applied to one, two, or three dimensions, given transport between segments. WASP4 can read output files from the link-node hydrodynamic model DYNHYD4, which predicts unsteady flow rates in unstratified rivers and estuaries given variable tides, wind, and inflow. A variety of water quality problems can

be addressed with the selection of appropriate kinetic subroutines. Two general toxic chemical modeling frameworks have been constructed from WASP-TOXIWASP (Ambrose et al. 1983) and WASTOX (Connolly and Winfield 1984, Connolly and Wise 1984). These separate frameworks are combined in WASP4. The WASP models are supported by EPA's Center for Exposure Assessment Modeling, Athens, GA.

TOXI4, subset of WASP4, simulates up to three interacting toxic chemicals and up to three sediment size fractions in the bed and overlying waters. First- or second-order kinetics can be used for all significant organic chemical reactions. Benthic exchange includes pore water advection, pore water diffusion, and deposition/scour. Net sedimentation and burial rates can be specified or calculated. An empirically based food chain model is linked to TOXI4 for calculating chemical concentrations in biota and fish resulting from predicted aquatic concentrations.

Hydrological Simulation Program FORTRAN (HSPF) is a comprehensive package for simulation of watershed hydrology and water quality for both conventional and toxic organic pollutants. HSPF simulates three sediment types (sand, silt, and clay) in addition to specific organic chemicals and transformation products of those chemicals. The reaction and transfer processes included are hydrolysis, oxidation, photolysis, biodegradation, volatilization, and sorption. Sorption is modeled as a first-order kinetic process in which the user must specify a desorption rate and equilibrium partition coefficient for each of the three solids types. Resuspension and settling of silts and clays (cohesive solids) are defined in terms of shear stress at the sediment-water interface. For sands, the capacity of the system to transport sand at a particular flow is calculated and resuspension or settling is defined by the difference between the sand in suspension and the calculated capacity. Calibration of the model requires data for each of the three solids types. Benthic exchange is modeled as sorption/desorption and deposition/scour with surficial benthic sediments. Underlying sediment and pore water are not modeled. HSPF is supported by EPA's Center for Exposure Assessment Modeling, Athens, GA.

The Sediment Radionuclide Transport Model - (SERATRA) framework (Onishi and Wise 1982) is a time-variable model for simulating radionuclides or organic chemicals in river systems. It solves the two-dimensional (vertical and longitudinal) advection-dispersion equation using finite element techniques for one chemical and three types of solids (sand, silt, and clay). Scour and deposition of solids are defined as in HSPF. The transfer and reaction processes included are hydrolysis, photolysis, oxidation, biodegradation, volatilization and sorption. Volatilization is computed from a user-specified oxygen transfer coefficient, limiting consideration of volatile organics to those which are liquid film controlled. Sorption is modeled as a first-order kinetic process for each of the three solids types. Benthic exchange is modeled as sorption/desorption and deposition/scour with surficial benthic sediments. Underlying sediment and pore water are not modeled. A similar one-dimensional (longitudinal) version for rivers (TODAM) and a two-dimensional (longitudinal and lateral) version for estuaries (FETRA) are also available from Batelle Pacific Northwest Laboratories, Richland, WA.

The Unified Transport Model for Toxicants - UTM-TOX (Browman et al. 1983) is an upgrade of the Unified Transport Model (UTM) originally developed to model heavy metal ions. It is a time-variable framework that includes atmospheric, terrestrial, and aquatic components. The aquatic component is designed to simulate streams and rivers. The transfer and reaction processes include sorption, volatilization, hydrolysis, biodegradation, and first-order photolysis. Sorption is described by an equilibrium partition coefficient. Sorbed phases are assumed unreactive (1982 version). UTM-TOX is available from Oak Ridge National Laboratories, Oak Ridge, TN.

METALS

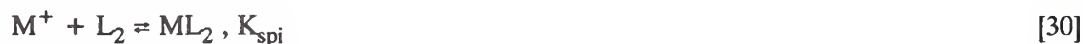
Metals are found naturally in the earth's crust. As a result of irrigation in some regions, metals may be solubilized and transported to surface waters. Steady or quasidynamic modeling approaches should be adequate if irrigation practices do not change.

Fate Processes

Upon entry to the surface water body, metal speciation may change due to complexation, precipitation, sorption, and redox reactions. Metals concentrations are further diluted by additional stream flow and mixing. Physical loss can be caused by settling and sedimentation, whereas a physical gain may be caused by resuspension.

Metal Complexation, Precipitation

Heavy metals can form complexes with liquids and can precipitate or dissolve



where M^+ = metal ion,
 L_1 and L_2 = liquids (such as carbonate, sulfide, or humate),
 ML_1 = soluble complex,
 ML_2 = insoluble complex,
 K_{ri} = equilibrium coefficient for reaction i, and
 K_{spi} = solubility product for reaction i.

Reaction times range from essentially instantaneous to thousands of years. At equilibrium, the distribution of metals among the possible complexes is controlled by the amount of metal and liquids present and the reaction coefficients and solubility products. In natural waters, sorption also affects the distribution by reducing the amount of metal available for complexation and precipitation.

Complexation reactions can affect transport by either increasing or decreasing the soluble fraction. Sometimes one chemical species is known to be much more toxic than another for a given heavy metal. This is especially important because some states and EPA have been moving toward "site-specific water quality standards," in which chemical speciation will be considered on a site-by-site basis. For example, a site that is known to have a great deal of naturally- occurring dissolved organics may not require as stringent a water quality standard because the dissolved organic material may complex the heavy metal and render it nontoxic to biota.

Sorption

Heavy metals frequently adsorb or "bind" to solid surfaces. The mechanism of sorption or attachment is via: 1) physical adsorption to solid surfaces, 2) chemical sorption or binding by liquids at the solid water interface, or 3) ion exchange with an ion at the solid water interface. In addition, if the heavy metal is complexed in solution by an organic liquid, it could sorb into the organic solid phase much like an organic pollutant. The mathematical formulation for describing the partitioning of the heavy metal between the solid phase and the aqueous phase is the same as for organic chemicals, except the K_{pi} is usually called the "distribution coefficient" for heavy metals (although it may be referred to as the partition coefficient or the binding constant in some cases). In most measurements and simulation models, all soluble complexes are lumped with the free ion to give the dissolved metal concentration. Precipitated metal is lumped with all sorbed species to give total particulate metal concentration. A spatially variable lumped distribution coefficient K_D

describes the two phases. There is no general consistency in reported K_D values for particular methods in the natural environment, so site-specific values should be used when possible.

Redox Reactions

Metals can change oxidation states through various oxidation and reduction reactions



where M^{++} = oxidized metal,
 M^+ = reduced metal,
 e^- = an electron, and
 K_{ri} = the equilibrium coefficient for reaction i.

Under some conditions, the kinetics of oxidation or reduction may be important to simulate.

Simulation Models

Two kinds of simulation models have been developed for metals in surface water systems. One addresses aquatic transport and fate, while the other addresses metals chemistry. The former are those general toxic chemical models that include benthic and water column compartments, partitioning, and particulate settling, resuspension, and sedimentation. These include MICHRIX, a steady state model for organics and metals; TOXIWASP, WASTOX, WASP3, WASP4, and HSPF, dynamic compartment models for organics and metals; SERATRA, FETRA, and TODAM, one and two-dimensional models for organics and metals; and UTM-TOX, a dynamic multimedia model for organics and metals. All of these have been discussed in an earlier section.

The second kind of simulation model addresses metals chemistry. Those developed for general application include organic and inorganic complexation, sorption, precipitation and dissolution, and redox reactions. These models are single compartment equilibrium models that calculate speciation for specified environmental conditions based on a set of thermodynamic constants. Environmental conditions, such as metal concentrations, liquid concentrations, pH, pE, and temperature, must be specified by the user. Thermodynamic constants are usually included in a database with the model. Examples of these models include MINTEQ (Felmy et al. 1984a and b) and MINTEQA1 (Brown and Shiao 1981); REDEQL and MINEQL; WATEQ (versions 1-4); and GEOCHEM.

Proper application of these models requires some specialized expertise because kinetic limitations at particular sites may prevent the thermodynamically possible reactions. Nevertheless, thoughtful application may reasonably describe the predominant metals species at a site and thus give useful insight into potential migration patterns and biological effects. For agricultural leaching problems, these models must be run in conjunction with one of the transport and transformation models described above.

MINTEQA1 (Felmy et al. 1984a and b; Brown et al. 1987) is a geochemical model that is capable of calculating equilibrium aqueous speciation, adsorption, gas phase partitioning, solid phase saturation states, and precipitation-dissolution of 11 metals (arsenic, cadmium, chromium, copper, lead, mercury, nickel, selenium, silver, thallium, and zinc). MINTEQA1 contains an extensive thermodynamic data set and six different algorithms for calculating adsorption. MINTEQA1 is supported by EPA's Center for Exposure Assessment Modeling in Athens, GA.

CHALLENGES AND RECOMMENDATIONS

Several challenges in the state of the art of water quality modeling are apparent.

Uncertainty

The composition of water quality models introduces and combines uncertainties from several sources: A recent review (Beck 1987) examines: (a) model structure, (b) model parameters, (c) propagation of prediction errors, and (d) experimental design to reduce critical uncertainties. In practical applications of WQ models uncertainty in input data is often a major limitation. In Beck's assessment there is ample evidence that "larger," more comprehensive models are easily capable of generating highly uncertain prediction of future behavior. Figure 7 gives the frame of reference for the analysis of uncertainty (Beck 1987). Aspects of model uncertainty are also addressed in stochastic modeling (see e.g. Reckhow et al. 1983). Model sensitivity to parameter variability and confidence levels of model outputs from probabilistic distributions of inputs are sometimes generated. Progress in this area will raise the reliability of models and help to identify "optimum sophistication in water quality modeling."

Toxic Substances

Current water quality concerns are with numerous toxic substances such as heavy metals (e.g. Hg, Pb, Cd) and chlorinated organics (e.g. DDT, PCB, dieldrin). The pathways and ultimate fates of these substances through ecosystems are often not fully understood, thus limiting the formulation of useful and reliable forecasting models at this time (Dolan and Bierman 1982; Thomann 1982). We need to improve our understanding and descriptions for processes affecting contaminant transport and fate, such as bacterial decomposition and partitioning of contaminants to solids. Additionally, work should focus on the transport of surface water contaminants to ground water. Verification of contaminant models has been greatly restricted by the expense of collecting appropriate data. Although confidence in these models will remain limited until they are properly validated, they are still very useful as a tool to assess research needs. Among the uncertainties are adsorption/desorption processes, interactions of organics and sediments, and surface chemistry. The formulation of adsorption isotherms frequently (Sweeney 1982) poses problems in model formulation. The problems apply to both suspended and deposited (bottom) sediments.

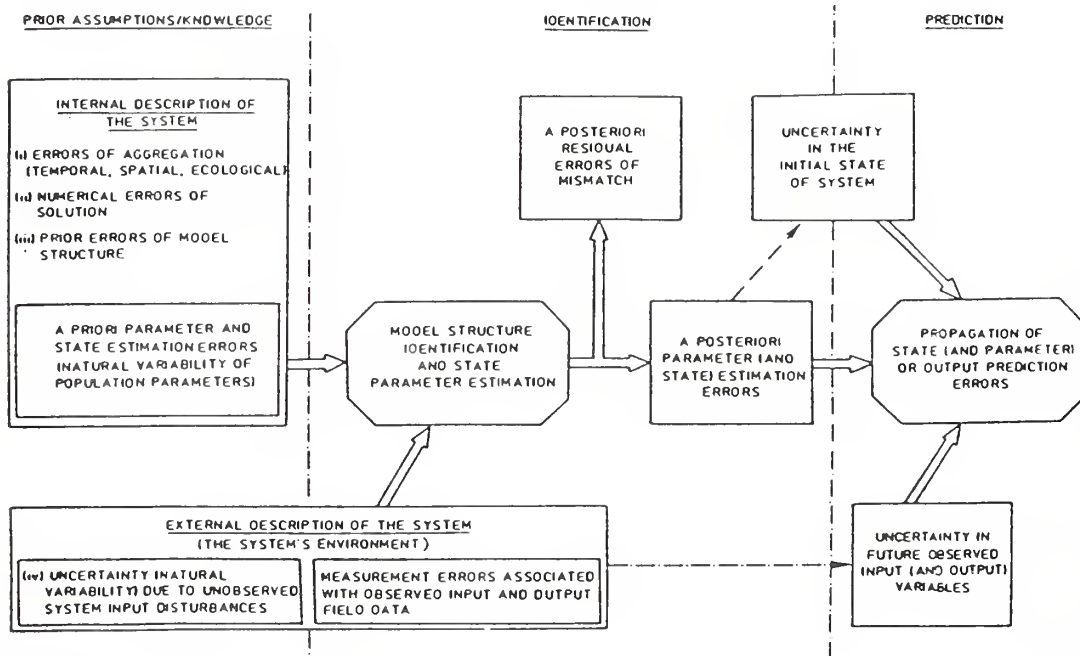


Figure 7.
Frame of reference for the analysis of uncertainty (from Beck 1987).

Acid Rain

Models that quantify the role of pH in aquatic ecosystems have been formulated (Schnoor 1987, Lang 1987, Weater et al. 1986) and are being refined. These models are intended to assist in the selection of appropriate acid rain abatement strategies. While basic chemical relationships to pH are known, the biological response can often not yet be quantified.

The greatest need in the area of conventional (DO/nutrient) water quality modeling is the development of reliable models that predict sediment diagenesis and fluxes to and from the bottom sediments. Water quality models will not be truly predictive until the bottom sediments are interactively coupled with the water column to provide time-varying SOD and nutrient fluxes that are predictable from previous conditions. Although some work has been started in this area (e.g. Hatcher 1986), there is still much study necessary. Proper sediment modeling will require an accounting of labile and refractory forms of particulate and dissolved organic matter in both the water column and bottom sediments.

Supercomputers

Capabilities for "number crunching" by supercomputers continue to rise dramatically. This appears to permit recourse to replace some empirical relationships with more fundamental ones, e.g. in flow simulation or in chemical partitioning. In the long term, most of the benefits likely will come from the ability to simulate long time frames in multiple dimensions, with the hydrodynamic and water quality models run on the same temporal and spatial scales. The biological parameters will probably continue to require numerous empirical relationships.

Artificial Intelligence

Spinoffs of artificial intelligence technology have resulted in the development of knowledge based and expert systems. Development of these systems for water quality models will improve user/computer interfaces and greatly reduce the difficulty of selecting and applying these models. Other related aspects are the development of pre- and post-processors, graphics, and other decision supports.

Microcomputers and PC's

Although the complexity of some WQ models makes their use for daily decision making impractical, managers should understand what is available and how it can be used. The EPA, through its water quality modeling program, and other agencies and universities can provide modeling packages and assistance. Some models are compact enough to be used on PC's and micros. User-friendly programs developed for personal computers permit decision makers to manipulate data bases and screen management options. This can be useful during managerial planning and policy discussions (Chapra and Canale 1987, Canale and Auer 1987).

Remote Sensing

Remote sensing offers intriguing possibilities for synoptic investigation of large areas (e.g. for reservoirs or watersheds). It appears that multispectral scanner information can be correlated with some water quality parameters collected on site (ground truth). If these correlations can be strengthened in further research, remotely sensed spatial distributions of surface water quality can be compared to model simulations. This can be useful for model validation, and also for updating of initial conditions for model simulations. The combination of remote sensing with water quality models may offer a reasonably inexpensive means to follow water quality evolutions in real time, e.g. for reservoir management.

Table 1.
Some Typical WQ Models.

Agricultural pollutants	All water bodies	Pond, lake, reservoir	River	Estuary
Sediment or total suspended solids	WASP4	CE-QUAL-R1 CE-QUAL-W2 RESQUAL II	HSPF SERATRA TODAM	CE-QUAL-W2 FETKA SSD-III
Organic waste and nutrients	WASP4- (EUTRO4)	CE-QUAL-R1 CE-QUAL-W2 MINLAKE	QUAL2E CE-QUAL-RIV1 HSPF	CE-QUAL-W2
Synthetic organics	EXAM-II WASP4- (TOXI4)		HSPF SERATRA TODAM UTM-TOX	FETRA
Metals transport	WASP4- (TOKI4)		MICHRIV HSPF SERATRA TODAM UTM-TOX	FETRA
Metals speciation	MINTEQA1 MINEQL WATEQ3 GEOCHEM			

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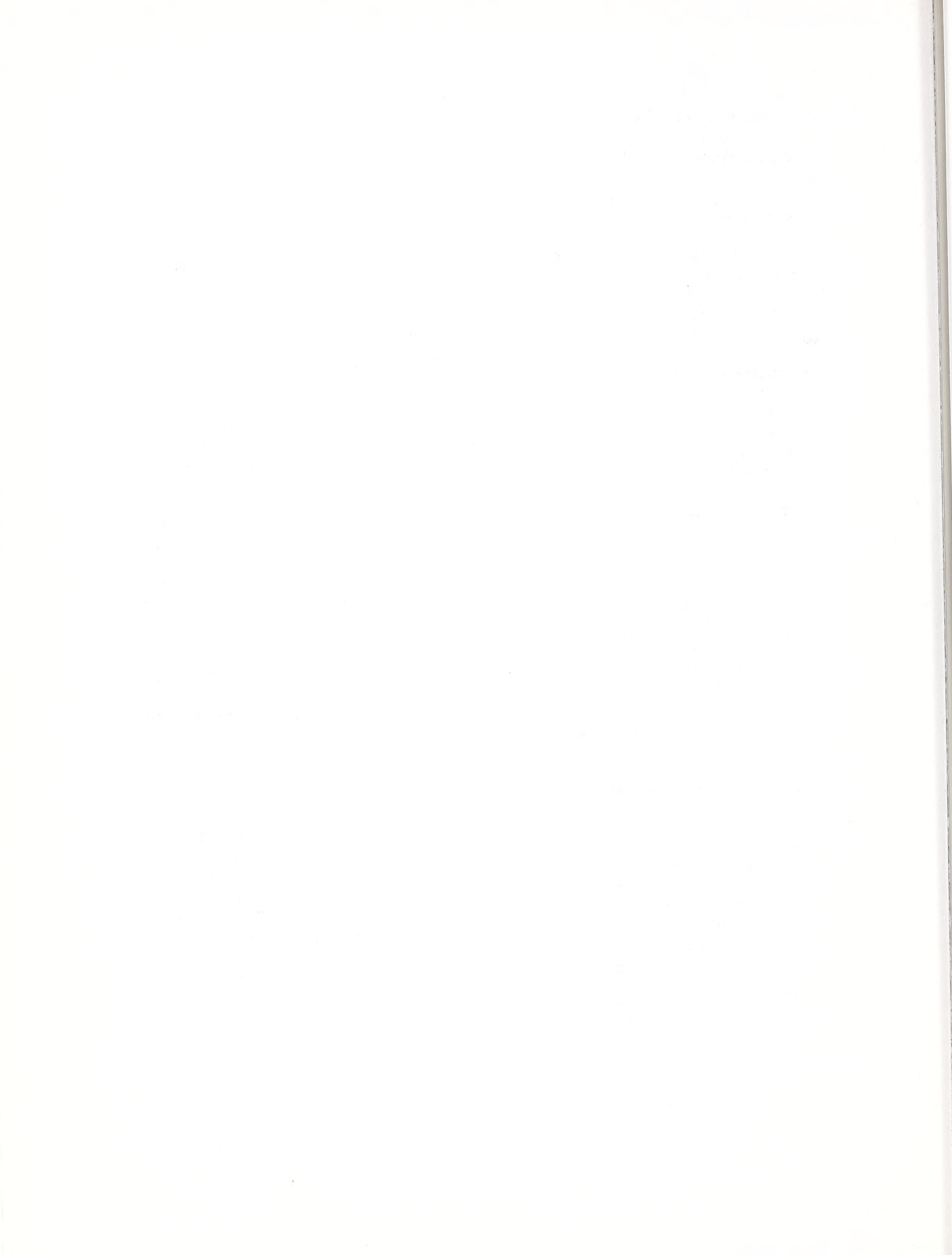
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WATER QUALITY MODELS: RIVERS AND RESERVOIRS

B. Henderson-Sellers¹, P.C. Young² and J. Ribeiro da Costa³

ABSTRACT

Both for day-to-day water quality management and for longer-term planning exercises, mathematical models can be useful tools to supplement insights gained from both field and laboratory observations. Models of a wide range of complexity are becoming increasingly available for water-quality studies and it is the selection, by the water quality manager, of the model most appropriate to a specific management goal that is perhaps one of the greatest problems.

The research areas in river and stream water quality modeling which require immediate attention appear to be the comparison and more detailed analysis of the similarities and differences in the attributes of the Advection-Dispersion Equation (ADE) and the Aggregated Dead Zone (ADZ) models for solute advection and dispersion in channels. Both model types have their merits and their relative practical utility will depend upon both the modeling objectives and the nature of the application.

The research areas in lake and reservoir water quality modeling which require immediate attention appear to be

- (1) the integration of continuously stirred reactor (CSR) and process models for biological and chemical variables with higher resolution (temporal and spatial) physico-chemical (largely thermodynamic and hydrodynamic) 1-, 2- and 3-dimensional models;
- (2) the need to formulate better diffusion parametrizations for throughflows (especially for low-retention-time reservoirs and pumped-storage reservoirs). At present mass conservation is included but, in general, the mixing feedbacks between an underflow or interflow and the otherwise lentic water body itself are excluded.

INTRODUCTION: MODELING CONCEPTS

Mathematical models can provide a useful tool to supplement insights gained from both field and laboratory observations. In river, lake and reservoir water-quality studies, there is an increasing availability of models of a wide range of complexity. For example, simple empirical models, such as assessments of lake trophic state (e.g., OECD 1982), may now be complemented by a range of computer simulation models. These continuous models may be characterized by the number of spatial dimensions, each represented by a number of physical, chemical and biological variables. Such computer-based mathematical modeling has increased in importance in recent years with the rapid evolution of computing power, both in terms of speed and storage capacity.

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In attempting to simulate water quality, we feel it is imperative that a multidisciplinary, integrated (systems science) approach be adopted. Not only is it vital to represent the chemical and biological variables on which water quality is based but it is also important that these complex processes be amalgamated with a representation of physical processes in such a way that the importance of the physical processes is acknowledged and feedbacks between biota and physical characteristics are possible. The most appropriate model is determined by many factors, from the evaluation of the current state-of-the-art models (often within a predetermined computational budget) to an appreciation of the implicit temporal and spatial scales which any modeler must have encapsulated within the numerical algorithm, and which, unfortunately, are not always 'visible' to the water quality manager (as model user). Indeed, it is not always the case that a complex and detailed model will provide the greatest advances in understanding; especially if input data requirements are large, the models need statistical estimation and/or a large effort to analyze the results.

A Model Hierarchy

A wide range of complexity exists in model formulation. This can be exemplified most simply, perhaps, in terms of the dimension of the model. Many of the more biologically and chemically orientated lake eutrophication models use the concept of the continuously-stirred reactor (CSR). This model, which is essentially a zero-dimensional lumped-parameter model, assumes that all state variables are homogeneously distributed throughout the water body (i.e., there are no spatial gradients represented). Consequently there is no possibility of understanding phenomena that are heterogeneous with depth or which occur on seasonal or diel (24-hour period) timescales; although the models may be very useful for longer timescale, year-to-year changes of, for example, phosphorus (e.g. Chapra 1977).

One-dimensional spatial models which represent the vertical direction in reservoirs and the along-reach direction in rivers are most evident in the literature. They have been used most extensively in both physical (e.g., reservoir stratification; stream pollutant advection) as well as chemical (e.g., dissolved oxygen) models; although in reservoir-ecosystem and eutrophication models (which attempt to describe the biota in more detail), vertical variability is seldom well resolved - at best only two or three layers in the vertical may be utilized.

Two-dimensional models are used to describe lateral and longitudinal variations in variable values but averaged over the depth. These may be useful for rivers and run-of-the-river reservoirs (e.g. Edinger and Buchak 1983) which have (i) a shallow depth and (ii) a strong throughflow, which tends to ensure the water is well-mixed in the vertical direction.

Three-dimensional reservoir models have been developed more recently, largely in hydrodynamic investigations of lake and reservoir currents (e.g. Paul and Lick 1981, Strub and Powell 1986). However, it is important to note that although the state-of-the-art in physical/thermodynamic models (Henderson-Sellers and Markland 1987) centers on 1-D models and in physical/dynamic models centers on 3-D models, there is an urgent need to fuse these apparently disparate approaches into fully three-dimensional representations of thermodynamics+dynamics+biochemical processes.

STREAMS AND RIVERS

It is axiomatic that polluting solutes which enter watercourses are transported downstream, where they affect the environment in various ways. The ability to describe and predict the effects of the transport processes on the distribution of solute concentrations is, therefore, of great importance for the investigation of problems such as estimating the assimilating capacity of rivers to receive urban and industrial effluents; assessing the ecological impact of the discharge of cooling water

from power stations; simulating the effects of proposed engineering works on mixing patterns; and predicting the passage of pollutant clouds through river systems. However, despite the success of numerical modeling studies of water movement in lakes, aquifers and estuaries which, in line with developments in computer power, have increasingly used complex time-dependent two- and three-dimensional models, improvements in the treatment of the apparently simpler problem of describing dynamic pollutant transport processes in rivers has tended to stagnate.

This situation has arisen in part from an over-confidence in the well-known Advection-Dispersion Equation (ADE) model (Fischer 1967, Fischer et al. 1979), which has provided the standard approach to water quality modeling in rivers over the last two decades. Recently, however, it has become more widely recognized that the theoretical justification for using the ADE is often confounded because of the limiting assumptions which underly its derivation (Chatwin 1980, Chatwin and Allen 1985). Although these restrictions had been noted previously (Fischer 1967, Sooky 1969, Fischer et al. 1979) and the model's limitations have been recognized from a practical point of view for some time (Thackston and Krenkel 1967, Day and Wood 1976), the ADE has continued to be popular in practical applications simply because no widely acceptable alternative had been proposed.

Largely in response to the practical limitations of the ADE model, a new approach to the water quality modeling problem has been evolving during the last few years based on the concept of "storage zones" or "dead zones", where solutes are differentially delayed in their transport down the stream channel (Thackston and Schnelle 1970). The most recent development of this kind is the Aggregated Dead Zone (ADZ) model (Beer and Young 1983, Young and Wallis 1986, Wallis et al. 1988) which shows a great deal of promise in practical application. In particular, experience shows that it is computationally much simpler than the ADE model and capable of providing a better description of the transport patterns observed in the real world.

Although we concentrate on the ADE and ADZ models in this section, other alternative mathematical representations have been proposed. Perhaps the two most promising of these alternatives are the delay-diffusion method (Smith 1981) and random walk based models (Sullivan 1971, Allen 1982). Interested readers are referred to these publications for further details and are strongly recommended to consult the recent review article by Chatwin and Allen (1985).

For the most part, we will consider the case of a conservative solute, so that the underlying physical mechanisms and basic principles of solute transport are not obfuscated by descriptions of non-conservative behavior. In some practical applications, however, it is clear that non-conservativity needs to be considered; in this case, the introduction of a simple decay non-conservativity into the ADZ model is obvious (Young and Wallis 1988) and the modification to include more complex chemical and biological interactions is straightforward (e.g., Beck and Young 1976, Beck 1983, Young 1983).

The Advection-Dispersion Equation

Observations reveal that, as a solute cloud is carried downstream in a water course, it disperses, with the cloud steadily lengthening and peak concentrations decreasing as the solute is distributed in the ever increasing volume of water. Although these effects are the result of a number of particular flow and mixing mechanisms, they are caused primarily by the interaction of two basic phenomena: differential advection and cross sectional-diffusion.

Open channel flows are shear flows--i.e., they support lateral and vertical gradients of longitudinal velocity. Therefore, solute is differentially advected (transported) downstream at the local flow velocity, with solute in the faster-moving water being carried downstream faster than solute in the slower-moving water. At the same time, solute is continually being distributed within the flow cross-section via a variety of different physical processes including transverse and vertical diffusion.

It is the interaction of differential advection with various cross-sectional diffusion processes which controls the dilution and longitudinal spreading of the solute cloud.

The classical mathematical treatment of the transport processes starts with the consideration of the conservation of mass of a solute within an infinitesimally small control volume (Fischer et al. 1979, James 1984). The net flux into the control volume comprises two parts: an advective component to represent advection of solute at the local longitudinal velocity and a diffusive component to represent transport of solute by molecular diffusion. Equations can be derived for the net fluxes in the longitudinal, lateral and vertical directions, and the sum of the three fluxes is equal to the rate of change of solute mass in the control volume.

Since river flows are almost always turbulent, it is necessary to incorporate the characteristics of turbulence into the analysis. It is recognized that instantaneous velocity components and solute concentrations exhibit random fluctuations about a mean value and that these create an additional diffusive transport of solute, usually termed turbulent diffusion (Hinze 1975). This is similar in form to molecular diffusion but, because the turbulent excursions occur over much larger distance scales than the Brownian motion responsible for molecular diffusion, turbulent diffusion is several orders of magnitude more effective in causing diffusive transport.

In the mathematical development of the ADE (as described in detail in Young and Wallis 1988) time averages are taken for each term over a period which appears to be long when compared to the turbulent fluctuations but short when compared to the timescale of changes in the mean components. This gives mean terms and second-order perturbation (Reynolds' stress) terms. It is usually assumed that these stress terms are represented by a product of the turbulent diffusion coefficient and the concentration gradient (Chatwin and Allen 1985):

$$-\overline{u'_i c'} = \epsilon_i \frac{\partial \bar{c}}{\partial x_i} \quad [1]$$

where u'_i = the i th component of the perturbed velocity,
 x_i ($i=1...3$) = the coordinate directions and
 ϵ_i = the i th component of the value of the turbulent diffusion coefficient for species c .

This gives the three dimensional turbulent diffusive equation*:

$$\frac{\partial \bar{c}}{\partial t} + \bar{u} \frac{\partial \bar{c}}{\partial x} + \bar{v} \frac{\partial \bar{c}}{\partial y} + \bar{w} \frac{\partial \bar{c}}{\partial z} = \frac{\partial}{\partial x} \left(\epsilon_x \frac{\partial \bar{c}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\epsilon_y \frac{\partial \bar{c}}{\partial y} \right) + \frac{\partial}{\partial z} \left(\epsilon_z \frac{\partial \bar{c}}{\partial z} \right) \quad [2]$$

which describes mixing due to turbulent fluctuations via a gradient diffusion process. The main justification for the use of equation 2 is that the variance of the concentration distributions grows linearly with time. This is precisely the property that Taylor (1954) showed applied to a cloud diffusing in a turbulent flow field within a pipe. However, the corollary to this is that equation 2 is only valid when the assumptions behind Taylor's analysis are satisfied.

In general, equation 2 cannot be solved analytically or numerically because neither the three-dimensional velocity field nor the distribution of the mixing coefficients is known. However, for the case of rivers in which solute transport eventually becomes a one-dimensional process, we do not need to use the three-dimensional form of the equation and instead can reduce it to a one-dimensional description by considering cross-sectionally averaged values of parameters which are functions of only the longitudinal coordinate and time. Integration of the general three-

*all symbols are defined in Appendix 1

dimensional transport equation over a constant cross section, A , yields an equation of the form (Fischer et al. 1979, Orlob 1983):

$$\frac{\partial \bar{c}}{\partial t} + \frac{\partial \bar{u}\bar{c}}{\partial x} - \frac{\partial}{\partial x} \left[D \frac{\partial \bar{c}}{\partial x} \right] \quad [3]$$

The value of D needs to reflect all the processes which affect the longitudinal spreading or dispersion of a solute cloud. The dominant mechanism producing longitudinal dispersion is normally assumed to be differential advection caused by the cross-sectional variation of the local longitudinal velocity. This component of the dispersion process is often called advective shear dispersion and its effects are limited by cross-sectional mixing mechanisms, which tend to break down the transverse concentration gradients it generates.

It is important to remember that this one-dimensional treatment of the spreading of a solute cloud retains the concept of a gradient diffusion-process and so the limitations of such a description still apply. These assumptions (Chatwin 1980, Chatwin and Allen 1985) are:

- (1) The solute cloud has been evolving for a sufficiently long time,
- (2) The turbulence is statistically stationary in time,
- (3) The velocity field is statistically steady, and
- (4) The solute is passive.

Under these conditions (discussed in detail by Young and Wallis 1988), equation 3 simplifies to the usual form known as the Advection-Dispersion Equation (ADE):

$$\frac{\partial \bar{c}}{\partial t} + \bar{u} \frac{\partial \bar{c}}{\partial x} - D \frac{\partial^2 \bar{c}}{\partial x^2} \quad [4]$$

because it is assumed that D , being dependent on flow conditions, will be constant.

The solution to equation 4 for input of an impulse of a finite mass of solute, M , with suitable choice for the origins of x and t (Chatwin 1970, 1971; Holley and Tsai 1977), is given by

$$\bar{c}(x,t) = \frac{M}{2A(\pi Dt)^{1/2}} \exp - \left[\frac{(x - \bar{u}t)^2}{4Dt} \right] \quad [5]$$

Although it is well known that this represents a Gaussian distribution in space, it is not always appreciated that, when it is viewed in the time domain (i.e., at a fixed longitudinal location), it yields a skewed distribution. This is inevitable, simply because a solute cloud will continue to evolve as it passes a fixed observation point.

It is also worth emphasizing now that equation 4 is no more general than equation 5, because the assumptions behind its derivation are such that deviations of concentration distributions from the Gaussian shape predicted by equation 5 are not described by equation 4 (Chatwin and Allen 1985). This was previously noted by Chatwin (1970, 1972, 1980) and it implies that if, in practice, concentration profiles are not Gaussian, then the conditions under which equation 4 is valid do not hold. This would imply that a different equation is required to describe the concentration profile.

Chatwin (1970, 1972) has argued that neither equation 4 nor 5 is valid until the asymptotic state is reached, (after the solute cloud has been evolving for a sufficiently long time). In practice,

however, this restriction appears to be less severe in some cases, and both equations may sometimes be applicable some time earlier (Fischer et al. 1979, Chatwin and Allen 1985).

Unfortunately, observations of dispersing solute clouds in rivers have revealed persistent deviations from the behavior predicted by the Fickian theory. In particular, measured concentration profiles rarely, if ever, attain a Gaussian shape. This is partly because it is usual to measure temporal rather than spatial profiles. However, even when this is taken into account, the skewness of the profiles persists and the Gaussian shape is not achieved (Day 1975, Day and Wood 1976, Nordin and Troutman 1980, Chatwin 1980). Other typical deviations are as follows:

- (1) The peak concentration reduces as t^{-n} where $0.5 \leq n \leq 1.4$ ($n = 0.5$ for Fickian theory);
- (2) The variance (whether spatial or temporal) grows as t^m where $1 < m < 2$ ($m = 1$ for Fickian theory) (Sabol and Nordin 1978, Liu and Cheng 1980); and,
- (3) Day (1975) and Beltaos (1980) report consistent deviations for the behavior of peak concentrations and variances with distance. There are two reasons for these deviations. Firstly, observations are rarely made at long enough times for the Gaussian distribution to evolve; and, secondly, to a greater or lesser extent, natural channels are non-uniform and this non-uniformity leads to more complete mixing and dispersion processes.

It is inevitable that most measurements taken during pollution incidents are carried out relatively close to the pollution sources because it is in these areas where the highest and, therefore, most environmentally damaging concentrations are likely to occur. Also the problems of logistics and instrument sensitivity often prevent tracer experiments being conducted over long enough time and distance scales. In other words, it may be that the Fickian theory appears never to apply, simply because measurements have not been taken at long enough times following introduction of the solute. Unfortunately it is exceedingly difficult to predict how long we would have to wait for the appropriate conditions to develop in natural channels because, to some extent, all natural channels are non-uniform and it is generally accepted that the presence of channel non-uniformity prolongs the time required for the conditions to materialize. Indeed, it may prevent them from developing at all (Valentine and Wood 1979b). In any case, a theory which demands such long periods of time for its efficacy is hardly likely to be very useful for many practical problems.

To summarize this situation, if the non-uniformity is relatively largescale, leading to significant changes in area, mean velocity and dispersion coefficient with longitudinal distance, then equation 5 can never hold (Chatwin 1980). Even if the non-uniformity is smallscale, it may cause sufficient changes in the cross-sectional distribution of velocity and boundary shear stress, such that the secondary flow pattern is constantly changing in the downstream direction. This would invalidate analyses such as Taylor's because a stable cross-sectional mixing mechanism would not exist long enough for the diffusive period to develop (Holly 1985).

Probably the most striking deviation between observations and Fickian theory is the additional skew in the measured concentration profiles. For temporal profiles this manifests itself as a sharper rise to the peak followed by a longer and more slowly decaying tail. Chatwin's (1980) method for estimating the dispersion coefficient illustrates this deviation well and is perhaps the best method for assessing whether or not the Fickian theory is applicable from an analysis of temporal concentration profiles (Chatwin 1975, Day 1975).

The Aggregated Dead Zone Model

The failure of the Advection-Dispersion Equation (ADE) to describe most observations in natural channels has stimulated workers either to modify the Fickian theory or to develop alternatives.

Many modifications to the Fickian models have been made (e.g. Liu and Cheng 1980). Of these, one approach which shows promise depends on the realization that "dead zones" play an important part in the dispersion process. These zones are traditionally associated with side pockets, bed irregularities, and roughness elements, which tend to create a relatively slowly moving region of flow around the periphery of the main flow. Solute which is entrained into these areas is released back into the main flow relatively slowly and at reduced concentrations due to the mixing mechanisms of the eddy-like flow structure contained therein. It is usual to assume that the exchange of solute between the main flow and the dead zones (and back again) is of the form of a simple first order mass transfer, such that the rate of change of concentration in the dead zone is proportional to the concentration difference between the dead zone and the main flow.

Various dead zone analyses (Valentine and Wood 1977, 1979a, 1979b; Thackston and Krenkel 1967; Thackston and Schnelle 1970; Sabol and Nordin 1978; Nordin and Troutman 1980; Bencala and Walters 1983; Legrand-Marcq and Laudelout 1985) have shown that dead zones can account for most of the observed deviations from traditional Fickian theory. In particular, they lengthen the times required for the diffusive or Taylor period to develop and for the concentration profiles to approach a Gaussian shape and, most importantly, they produce long tails on the profiles, such as those encountered in practice.

Until recently, most dead zone models have been based on an extension of the ADE model, in which the dead zones are modeled explicitly as a second-order differential equation adjoined to the classical partial differential equation (equation 4) of the ADE. In a more radical innovation, Beer and Young (1983) have suggested that the dead zone dispersion often so dominates the turbulent shear flow dispersion of the ADE model that most of the dispersion could be attributed to the aggregated effect of dead zone processes alone. The resulting aggregated dead zone (ADZ) model has a lumped-parameter ordinary differential equation form which appears often to offer considerable advantages over the distributed-parameter partial differential form of the ADE model. Not only is such an inherently stable, discrete time solution easier to formulate, but the ADZ model appears better able to describe observed patterns of dispersion at all time scales.

The success of the ADZ model in describing observed solute concentrations has stimulated the need to establish a link between the ADZ model parameters and conventional open channel flow parameters. A recent study (Young and Wallis 1986, Wallis et al. 1988) has demonstrated the utility of the ADZ in a range of stream channels in N.W. England. Figure 1, for the River Dunsop, is typical of the results obtained in this study and demonstrates the remarkable ability of the model to explain closely the observed tracer concentrations in a natural channel.

The ADZ is different from the ADE model in a number of ways:

- (1) firstly, as we shall see, it is a lumped rather than a distributed-parameter model;
- (2) It assumes, as we have noted previously, that the dead zone dispersion so dominates the turbulent shear flow dispersion of the ADE model that most of the observed dispersion can be attributed to the aggregated effect of the dead zone processes alone.
- (3) The idea of "data-based modeling" (or statistical calibration) is introduced by Beer and Young (1983) as a rigorous discipline by which to first "identify" the most appropriate model structure on the basis of the observed changes in solute concentration (e.g., as obtained from a tracer experiment); and then to "estimate" statistically the parameters which characterize this "best" model.

The aggregated dead zone concept does not easily subscribe to the distributed-parameter partial differential equation formulation because it represents the lumped effect of all dispersive processes in any given length of channel, as modeled by one or more (depending on the reach characteristics) aggregated dead zones; in other words, the ADZ model is naturally a lumped-

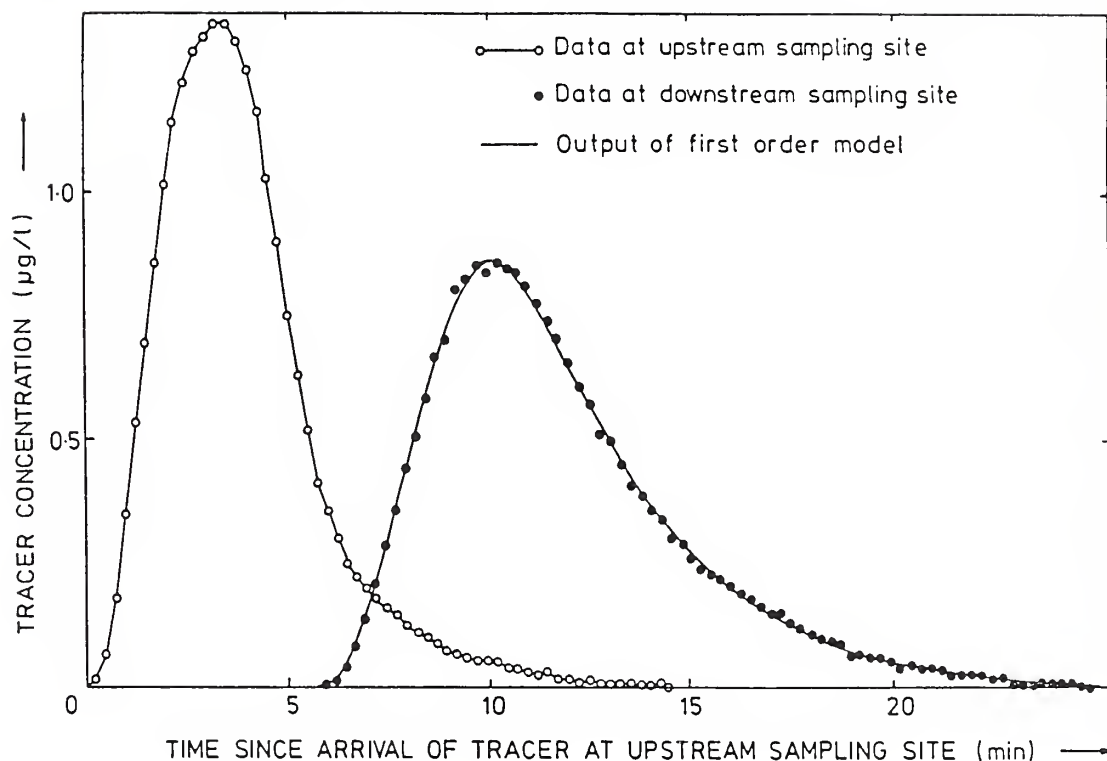


Figure 1.
Typical ADZ modeling results for the River Dunsop.

parameter concept at the reach level and so an ordinary differential representation offers the simplest prospect of describing the overall dispersive effect of the reach.

Since the ADZ model regards dead zone processes as being the major physical cause of dispersion in natural channels, it is sensible to assume initially that the simplest dynamic structure necessary to describe a whole reach will be the same as that required to describe a single dead zone. Let us consider, therefore, a single dead zone with volume V in a flow field with discharge Q . Assuming a conservative solute with complete and instantaneous mixing throughout the dead zone, a simple dynamic mass balance similar to that used in CSR analysis yields the following ordinary differential equation

$$\frac{d[V(t)c_o(t)]}{dt} = Q(t)c_i(t) - Q(t)c_o(t) \quad [6]$$

Rate of change of mass	Mass in per unit time	Mass out per unit time
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where $c_i(t)$ is the concentration of solute entering the dead zone and $c_o(t)$ is the concentration within the dead zone which, because of the complete mixing assumption, is equal to the output concentration.

For steady flow, with both V and Q constant, equation 6 simplifies to the following form:

$$\frac{dc_o(t)}{dt} = -\frac{Q}{V} c_o(t) + \frac{Q}{V} c_i(t) \quad [7]$$

which is a simple first order differential equation describing the relationship between the changes in concentration of the solute within the dead zone to the concentration gradient between the dead zone and the input ($C_i(t) - C_o(t)$). In this equation, the dispersive effect of the dead zone is revealed by the response of $c_o(t)$ to an impulsive input of solute at the input, i.e., with $c_i(t)$ specified as a Dirac delta function at $t=0$ and zero for all other time. It is easy to show that this unit impulse response is given by

$$c_o(t) = \alpha \exp(-\alpha t) \quad [8]$$

where

$$\alpha = \frac{Q}{V}. \quad [9]$$

In other words, the impulsive input is dispersed to yield a concentration profile at the output of the dead zone which decreases exponentially with time following an initial sharp rise.

Equation 7 represents a model for the dispersive behavior of the solute in a single dead zone within a given length or reach of the channel. In order to describe the dispersive process over the whole reach, we now make a crucial assumption (Beer and Young 1983): that the aggregated effect of all such dead zones in the reach can be described by an equation of a similar form to equation 7, but with the volume V replaced by an effective, and much larger, Aggregated Dead Zone (ADZ) volume, V_e . So far, research has not established the nature of the underlying aggregative mechanism which would justify this assumption in theoretical terms, but its practical justification is revealed in the results of the field experiments discussed by Wallis et al. (1988). However, theoretical studies which support some aspects of the ADZ modeling within the more traditional fluid dynamics context have appeared recently (Smith 1987, Purnama 1988).

In order to complete the ADZ description at the reach level, it is also necessary to model the advective properties of the channel; indeed, advection often dominates dispersion in its overall effect on the solute transport in certain channels. The physical effect of advection can be considered simply as the introduction of a pure time delay of τ time units between the upstream and downstream concentration-time profiles; where τ is the time taken for the leading edge of the solute cloud to be advected through the reach.

With the above modifications, the elemental ADZ model at the k th reach of a channel system can be written in the form

$$\frac{dc_k(t)}{dt} = -\alpha c_k(t) + \beta c_{k-1}(t-\tau) \quad [10]$$

where c_{k-1} is the solute concentration measured at the output of the previous, or $(k-1)$ th, reach. In the conservative situation

$$\alpha = \beta = 1/T_R \quad [11]$$

with $T_R = V_e/Q$ representing the ADZ residence time, the time constant associated with the solute's passage through the ADZ element.

In the non-conservative situation, it is necessary to consider the effect of the decay process during the time period associated with the advective time delay, as well as its effect within the ADZ (see Young and Ribeiro da Costa 1985). This gives a non-conservative ADZ model in which the coefficients α and β are modified in terms of a decay rate coefficient, k

$$\alpha = k + \frac{1}{T_R}; \quad \beta = \left(\frac{1}{T_R} \right) e^{-k\tau} \quad [12]$$

In a similar manner, the ADZ model can be extended to allow for chemical/biological interaction assuming either linear or nonlinear kinetics. In general, such extensions require the formulation of several interconnected state equations, each posed in the same general form as equation 10, but representing a different chemical or biological variable. Additional terms on the left-hand side can then be introduced to represent the dynamic mass balance of the variable and any interactions with the variables described by the other equations. The result is an interconnected set of differential-delay equations which represent the behavior over the reach in question and can be solved on a digital computer in the normal manner. However, as we point out below, it is usually advantageous to formulate the model in these continuous-time terms and then transform them to their discrete-time equivalent. A typical and early example of this general approach is the BOD-DO model of Beck and Young (1976). More recent discussion which relates to this general approach is available in Beck and van Straten (1983).

The number of ADZ elements required to model any channel system will depend very much on the channel length and the associated reach characteristics. In general, therefore, it is necessary to consider a more general model which comprises a number of ADZ elements, each described by a differential-delay equation such as equation 10 or an equivalent set of interconnected state equations, either in some physically appropriate series or possibly in series/parallel combination. Having constructed such a network ADZ model, it is then straightforward to introduce point or diffuse pollutant inputs at the reach boundaries. This approach is the basis for sophisticated, visual-interactive ADZ computer models being developed in studies of the water quality in the River Ave of Northern Portugal (e.g. Young and Ribeiro da Costa 1985).

In order to explore this further, however, it is convenient to consider the discrete-time version of equation 10. Such a formulation, which can be compared to a finite difference numerical solution of equation 10 but will normally be of much lower dimension, is not only preferable when dealing with sampled data, but it also allows for the application of sophisticated methods of recursive time-series modeling (Young 1984), which are normally posed in similar discrete-time terms (Young and Wallis 1985, 1986, 1988).

The use of recursive time-series methods to estimate the ADZ model parameters has several advantages. Firstly, it allows the modeling to be placed within a stochastic setting, so permitting its use in probabilistic simulations and forecasting applications. Secondly, it means that the recursive parameter estimates can be examined to investigate possible non-stationarity and, if necessary, used within an "adaption" forecasting context (e.g., Young 1987). Finally, and of particular importance in the present context, it provides an objective method for defining the "structure" of the ADZ model appropriate to a particular channel length; i.e., the number of ADZ elements such as equation 10 required to characterize the transport and dispersion dynamics adequately.

Statistical model structure identification is not common in the modeling of pollutant transport and dispersion but it is potentially of great importance in removing some of the subjectivity that often characterizes the modeling of complex environmental phenomena. For example, in the case of the River Conder, this identification procedure has revealed second order ADZ reach models which can be interpreted physically in terms of parallel, two-layer flow (see Wallis et al. 1988).

One advantage of the ADZ approach is that it helps to provide a reasonable model for the underlying solute transport and dispersion characteristics of the river; characteristics which are so important in defining the dynamics of water quality and yet can be reasonably validated by planned tracer experiments. It is well known that such planned experimentation is not so straightforward in the case of more general chemical and biological water quality variables. The models for these need to be calibrated and validated by reference to monitored data, normally collected during the "normal operation" of the river, without resort to any special, planned input perturbations. By utilizing the ADZ approach, therefore, the modeler can introduce the more speculative modeling of these other non-conservative and interactive water quality variables within the physical framework of a well validated ADZ transport-dispersion model. This is particularly important at medium-to-high flow rates, since it is these physical aspects of the reach behavior which have a dominant influence on the temporal variations in water quality over the reach.

Finally, it is important to note that the experimental evaluation of the ADZ model (Young and Wallis 1986, Wallis et al. 1988) has revealed a number of important empirical and practical aspects of the model. These findings are very important in practice, since they help to generalize the ADZ model parametrization over a wide range of discharge rates. They thus simplify both planned experimentation and associated statistical model calibration. Perhaps the most important of these results are illustrated in figures 2 and 3: these show, respectively, the variation in residence time, T_R , and advective time delay, τ , with discharge; and the relationship between the "dispersive fraction", $D_f = T_R/\bar{t}$, and discharge, where \bar{t} is the mean travel time for the reach. These results were obtained for the River Conder but are typical of those obtained for other rivers in the study.

The dispersive fraction, D_f , describes the time the tracer appears to spend being dispersed in the reach, as a fraction of the total time it resides in the reach. Furthermore, since it is also directly equivalent to the ratio of the effective volume to the reach volume, V_e/V , it can also be interpreted as the fractional volume of the reach that appears responsible for dispersion. While the pattern of variation of T_R and τ with discharge is reasonably predictable, the relative invariance of D_f is both surprising and significant. In particular, it is always satisfying if such an invariant parameter can be observed in scientific investigations, since the parameter can then be used to characterize the physical system; in this case, the nature of the stream channel. For example, the field experiments so far indicate that D_f ranges from 0.3-0.4 for natural channels, but is significantly lower at 0.1-0.2 for artificial channels. In addition, if the discovery of this discharge-invariant parameter is confirmed by subsequent experiments on a wider range of stream channels, it suggests that a small number of tracer experiments (or even a single experiment in the ideal case), when combined with estimates of the mean travel time based on the hydraulics of flow, will yield sufficient information to "calibrate" the ADZ model for a wide range of discharge, and so further enhance the model's utility in practical terms. Further evaluation of the ADZ model in this regard is proceeding in collaboration with the North West Water Authority, Yorkshire Water Authority and the UK Water Research Center.

Summary

The ADZ approach to modeling the advection and dispersion of a solute in a river system is still comparatively new and the results from this approach are encouraging. In particular, the model appears to be able to describe, with very few parameters and quite remarkable accuracy, the solute concentration profiles measured in practice. Moreover, the main ADZ model parameters have direct, albeit somewhat unconventional, physical significance, show variations with discharge that make good physical sense and are related by the "invariant" dispersive factor, D_f .

The ADZ model appears to offer three significant advantages over the conventional advection-dispersion equation (ADE). Firstly, it is simpler in algorithmic and modeling terms; secondly, it is often capable of more accurate descriptions of observed dispersion events at all time scales; and finally, it can be calibrated using statistically-based procedures which objectively identify the

number of ADZ elements appropriate to a given length of channel and provide measures of the uncertainty associated with the model parameters which can be used in later forecasting applications (Young and Wallis 1985, Young 1986, Young 1987, Beven et al. 1987). Nevertheless, before the model can be used with confidence, more research will be needed to correlate the ADZ parameters with a wider range of channel and flow characteristics.

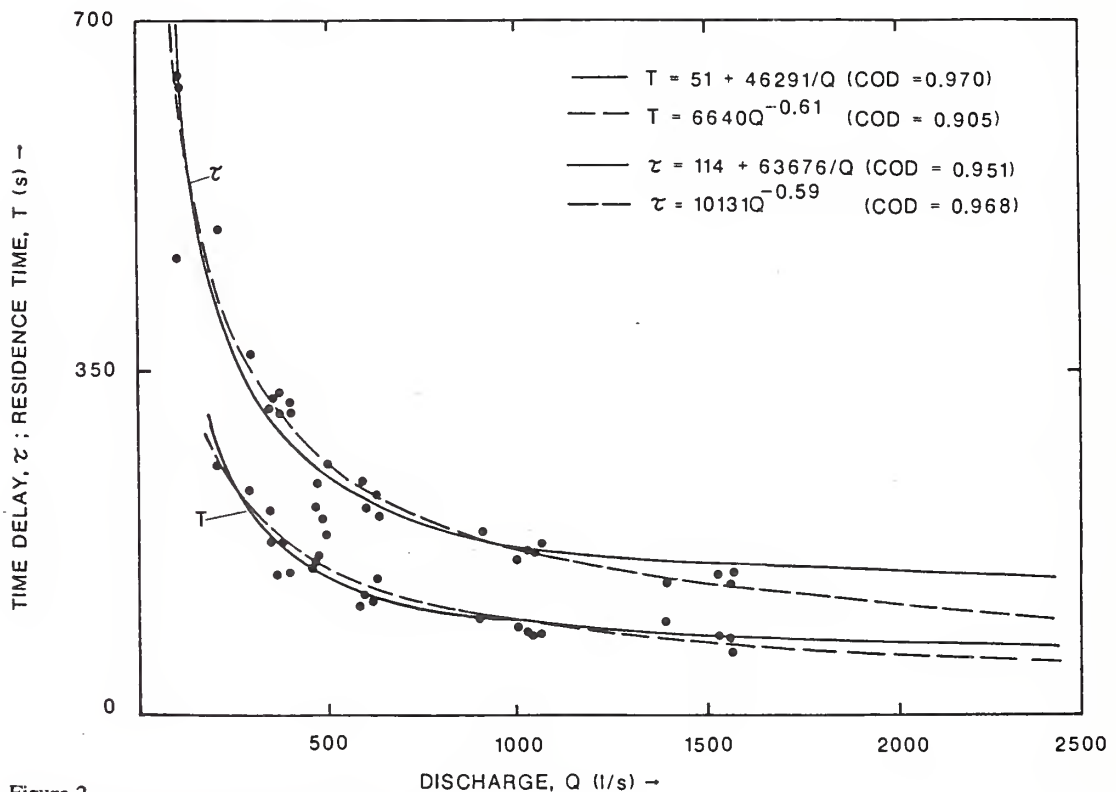


Figure 2.
Variation of the ADZ residence time, T_R , and advective time delay, τ , with discharge, Q , for the River Conder.

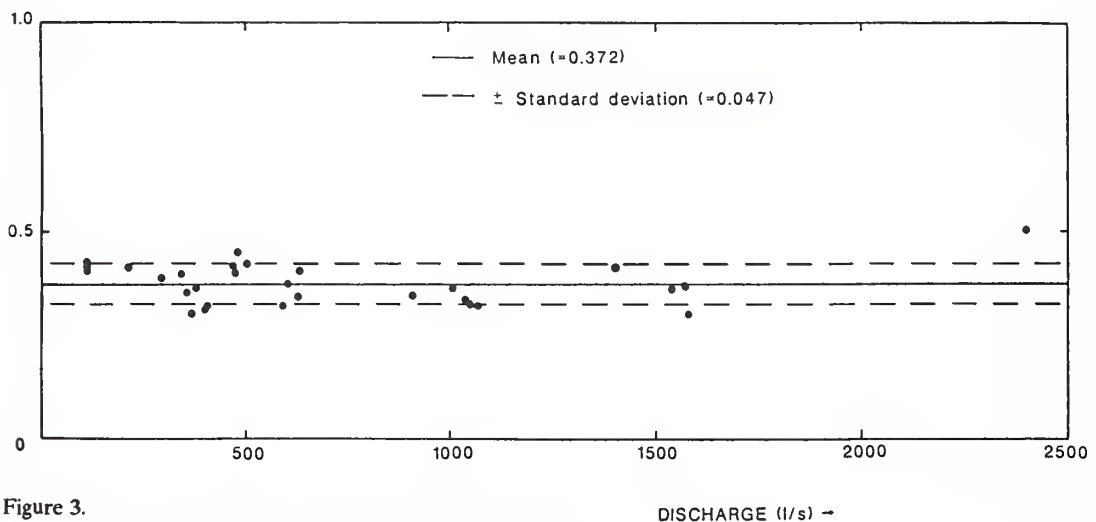


Figure 3.
The dispersion fraction $D_f = T_R / \bar{l}$ as a function of discharge for the River Conder.

RESERVOIR MODELS

Stratification Modeling

In lentic water bodies (lakes and reservoirs) of all sizes, the temperature patterns and the way they change over both seasonal and diel (i.e., over a 24 hour period) cycles are determined by a wide range of influences. Under different circumstances, these forcing processes may include imbalance in the surface energy budget, penetration of shortwave radiation, convection, turbulent mixing, advection, currents and physico-chemical characteristics of the water (e.g., turbidity, salinity). Knowledge of the temperature characteristics of water bodies may be of importance directly (e.g., controlling the temperature, and hence acceptability, of potable water in reservoirs), in the influence on chemical transports (e.g., in eutrophication studies; Gulliver and Stefan 1982) and as a component part of a larger scale model (e.g., global climate modeling; Semtner 1984). Mathematical models are available on different time and space scales as aids to understanding the complex interactions occurring between these various processes.

The normal equations used to describe the vertical profiles of temperature and velocity in a water body have been stated or derived by many authors. The equations may be expressed in vector form (e.g. Niller 1975) or component form (e.g. Mellor and Durbin 1975). Neglecting the horizontal advection terms (in contrast to the approach taken in river modeling), the vector form is

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{f} \wedge \mathbf{v} = - \frac{\partial}{\partial z} [\overline{\mathbf{v}' \mathbf{w}'}] - \frac{\mathbf{F}}{\rho_0} \quad [13]$$

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial z} [\overline{\mathbf{w}' T'}] = \frac{Q_*(z,t)}{\rho_w c_p} \quad [14]$$

The methods of solution which are discussed briefly below refer to the different methods of closure of these equations (essentially via the correlation terms $\mathbf{w}' \mathbf{v}'$, $\mathbf{w}' T'$), the neglect of differing energy transfer processes as well as differing parametrizations of the terms retained. The mode of closure selected can be used to divide the models into those using an eddy diffusion closure scheme (e.g. Mellor and Durbin 1975, Henderson-Sellers 1985); and those in which closure is expressed in terms of the rate of descent of the thermocline, given simply as the rate of change of mixed layer depth. However, a more useful division is between differential models which solve the primitive equations in a multi-level finite difference scheme and bulk or integral models which make an a priori assumption about the existence of a homogeneous mixed layer (ML). Consequently differential models are able to predict the existence and depth of a mixed layer; and, in contrast, the assumed existence of this homogeneous mixed layer by the bulk model permits the equations to be simplified by integration over the depth of the ML. The characteristics of the ML are thus represented by a single equation, which decreases the computational time required for solution at the expense of resolution within the ML; for example, they may not be as able to represent biological parameters, such as diel vertical migration of blue-green algae (Reynolds and Walsby 1975). These model types can be exemplified by (i) the mixed layer model DYRESM (e.g. Spigel and Imberger 1980) and (ii) the eddy diffusion model EDD1 (Eddy Diffusion Dimension 1) (Henderson-Sellers 1988). These two types of models have been developed in parallel for some years and both have been shown to be more than adequate for simulating a wide range of lakes and reservoirs. Clearly a direct comparison of these models, already undertaken analytically (Henderson-Sellers and Davies 1988), needs to be repeated numerically using common data sets (cf. comparable oceanic testing of Martin 1985).

Mixed layer (ML) models. Simplifications may be made within the framework of the bulk ML models, leading to the identification of the DIM (dynamic instability model - e.g., Pollard et al. 1973) and the TEM (turbulent erosion model - e.g. Kraus and Turner 1967) - see figure 4.

These different approximations are in fact valid over different timescales (e.g. Niiler 1977, de Szoeke and Rhines 1976). Furthermore it is a common assumption (e.g. Niiler 1975) that the waters underlying the interface are a "quiescent abyss", i.e. no energy "leaks" into these waters from above (nor also by direct radiative penetration). It is also worth noting here that such restrictions have never been necessitated in the alternative (eddy diffusion) approach to mixed layer modeling.

Modeling approaches to thermal stratification which utilize the integral energy (mixed layer) concept differ in the way they treat the parametrization of each of these different sources of turbulent kinetic energy (TKE) (including the possible neglect of some of the terms) and in how the net TKE is partitioned between enhancing waves, currents and the descent of the thermocline.

As noted by Niiler and Kraus (1977) that, while the specification of the mixing length scale is the most arbitrary part of a turbulent diffusion closure model (e.g. Mellor and Durbin 1975), the most arbitrary part of an integral mixed layer model is in the specification of the dissipation term.

Although much of the early work in mixed layer models was ocean-oriented, lake ML models are essentially TEMs. Since it is normally intended to utilize such models to simulate seasonal time scales and longer, this is appropriate. For example, Stefan and Ford (1975) derived their lake model by considering that input kinetic energy (from the wind) will change the potential energy of

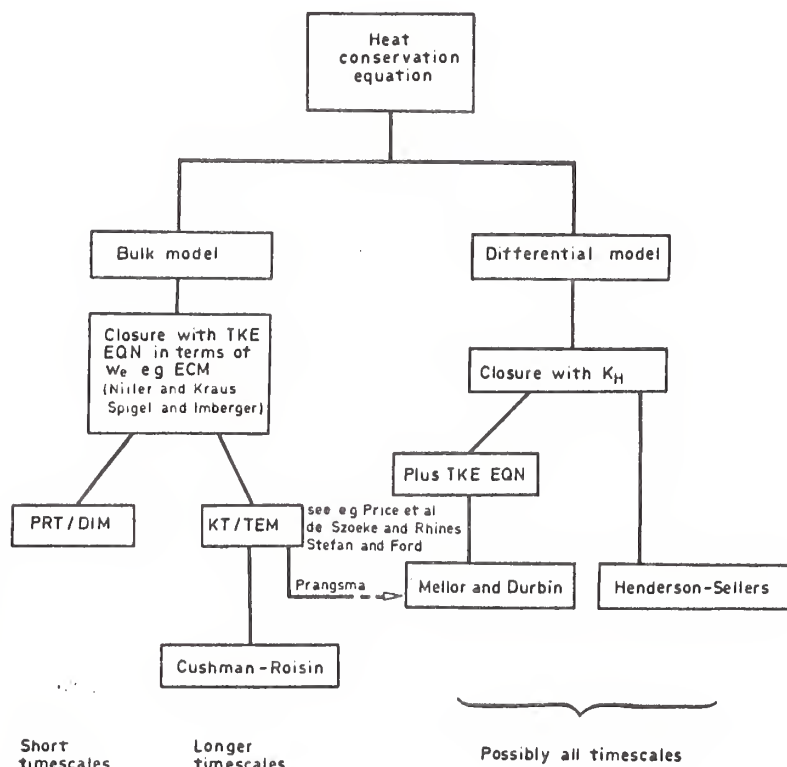


Figure 4.
Flow chart describing various forms of mixed-layer and stratification models, differentiating between ECM, DIM, TEM and differential models.

the water column or will be dissipated. A similar approach is discussed by Sherman et al. (1978) and Imberger et al. (1978) but using four empirical constants. Spigel and Imberger (1980) synopsized this in the form of an energy conservation model (ECM), expressed in finite difference form.

Differential models. Eddy diffusion models of the thermocline start with the same set of equations 13 and 14 but parameterize the Reynolds' stress terms using an eddy diffusion coefficient, K . This closure can be undertaken at any one of a hierarchical set of "levels" (Mellor and Yamada 1974). At the lowest level, a relationship is invoked between the stress terms and the eddy diffusion coefficients of the form of equation 1 for heat and momentum in the vertical direction; and it is this formulation that was originally applied extensively. Differences between models relate to the mode of parametrization of the value of the eddy diffusion coefficients for heat and momentum as functions of both the ambient meteorological and oceanographical conditions and as a function of the stability (e.g., Rossby and Montgomery (1935); Munk and Anderson (1948); Mellor and Yamada (1974)). These arguments permit the dynamics and thermodynamics to be effectively decoupled so that equation 14 is solved in the form

$$A(z) \frac{\partial T}{\partial t} - \frac{\partial}{\partial z} \left[A(z)(\alpha_H + K_H) \frac{\partial T}{\partial z} \right] + \frac{(\partial/\partial z)(A(z)\phi(z))}{\rho_w c_p} \quad [15]$$

where the molecular diffusivity of heat, α_H , is included so that, for low wind speed or large depth situations, a minimal diffusion is predicted. The cross-sectional area term, $A(z)$, must be included for lake basins, while in the ocean a water column is usually considered whereby $A(z) = \text{constant}$, thus permitting simplification of equation 15. Using representations for the turbulent diffusion coefficients there is no need to specify the TKE, as in the Mellor and Durbin (1975) diffusion model, since these forms of closure for K_H are sufficient.

Availability of Stratification Models

Software packages for thermal stratification have not been made generally available but can often be obtained by direct contact with the authors. (For details of sources, see the cited papers themselves, e.g., Semtner 1984, Mellor and Durbin 1975, Henderson-Sellers 1985, Pollard et al. 1973, Niiler and Kraus 1977, Stefan and Ford 1975, Imberger et al. 1978, Price et al. 1986, Harleman 1982). In some cases, the original stratification model codes have been later incorporated into larger models. For example, the model CE-THERM (Environmental Laboratory 1982) is part of CE-QUAL-R1 (a lake water quality model of the mixed layer type); the model of Stefan and Ford (1975) is now part of the University of Minnesota model RESQUAL II. Other models known by acronyms are DYRESM (Spigel and Imberger 1980) and EDD1 (Henderson-Sellers 1988). The majority of ocean numerical models would appear to be recoding of earlier analytical models - again individual authors should be contacted regarding code availability.

Model Transferability

Existing stratification models have often been designed for a single application and hence include tuning to one particular data set (e.g. Johnson and Ford 1981). To be of wider applicability, it is vital to include a conceptual framework for such a model. One technique available is to utilize observational data sets from a wide range of sites (cf. preliminary results given by Henderson-Sellers and Reckhow 1988) so that each parameter may be assessed for its significance and also for its sensitivity to perturbations which may result from deficiencies in either forcing data or in the model parametrizations. For example, the effect of flood or drought events is difficult to assess from a U.K. data base because of the rarity of such events; errors in cloud cover are likely to be less important in the U.K. than in the subtropics where the absolute magnitude of the annual incident radiation is considerably higher so that a small error in cloud cover estimation can result

in a significant error in calculation of the surface heat flux which is the major energy source for the reservoir energy budget (McGuffie and Henderson-Sellers 1988).

Existing models of thermal stratification in lakes have often been designed for a single application/case study and consequently frequently include calibration coefficients to permit simulation of any specific data set. For example, CE-QUAL-R1 (Environmental Laboratory 1982) can only be applied directly to the single lake for which they were originally devised, or to similar lakes following either recalibration (e.g. Johnson and Ford 1981) or indeed reformulation of the model itself (Wlosinski and Dortch 1985). This model (which is part of the larger water quality model CE-QUAL-R1) has seven tuning (or calibration) coefficients within its structure (Waide, J., p.c. 1982). To implement the model it is first necessary to evaluate these seven coefficients by "trial and error" on a single year's data (a "learning set"). When the seven coefficients have been selected, then a second year's data are used to verify that the model has been relatively well construed for this particular lake. Further simulations may then be possible prognostically, although whether such models can ever predict for conditions beyond their original tuning must remain severely in doubt. The original attempt at transferability of this model was from DeGray Lake in Arkansas (the calibration lake) to Greeson Lake in the same state (Johnson and Ford 1981). More recent experiments have utilized data from Eau Galle reservoir in Wisconsin. For pumped storage investigations, Carters Lake in Georgia has been simulated (Wlosinski and Dortch 1985). These authors found that when applying the model to Eau Galle Reservoir it was necessary to add a subroutine for macrophytes and to extend the description of algae and of diatom photosynthesis. For the description of inflows it was found that "To better represent these flows, the code was changed ... so that the inflow or outflow was not allowed into those layers representing the borrow pit". Following the recalibration, it was suggested that "all of the major dynamics at Eau Galle were satisfactorily predicted, except for the disappearance during one sampling period of a metalimnetic maxima for nitrite plus nitrate nitrogen".

One model which is intended as a generalized model, applicable to a wider data base *without* tuning or recalibration, is the model EDD1 (Henderson-Sellers 1985, 1988). Preliminary results (Henderson-Sellers and Reckhow 1988) based on three separate climatic regimes (north temperate maritime (U.K.), north temperate continental (Ontario) and sub-tropical (South Africa)) suggest a potential usefulness to this approach. Results from a larger number of contrasting lake sites are currently being analyzed (Henderson-Sellers, B., in preparation).

Surface Energy Forcing

The water body heats up/cools down (increase/decrease of stored thermal energy) largely by atmospheric forcing (including solar radiation). Typical total daily heat input to a water body may be of the order of 2.5 MJ m^{-2} (an average energy flux of the order of 25 W m^{-2}) at latitudes of approximately 50°N . This is composed of a range of radiative and non-radiative heat fluxes (e.g. longwave atmospheric radiation, shortwave solar radiation, evaporation), all of which have magnitudes of tens or hundreds of watts per square meter. Consequently it is necessary to evaluate the surface energy budget (SEB) in order to assess the available energy both at the surface and at depth.

Almost all energy exchanges at the surface occur within the top few millimeters (McAlister and Macleish 1969) and can thus be considered as occurring at the air-water interface, the exception being that a portion of the shortwave radiation penetrates this surface layer. It is important to determine fairly accurately the total heat budget of the lake, as well as the feedbacks associated with the surface energy fluxes. The net available energy, ϕ_N , can be given as the sum of the non-reflected incoming shortwave radiation, ϕ_0 , the non-reflected incoming atmospheric longwave radiation, ϕ_{H} , the outgoing longwave radiation, ϕ_{ro} , the evaporative energy flux, ϕ_e , and the

convective (or sensible) heat loss, ϕ_c . (In this calculation the heat flux associated with precipitation is negligible because there is no phase change). Thus

$$\phi_N = \phi_0 + \phi_{ri} - \phi_{ro} - \phi_e - \phi_c \quad [16]$$

The portion of the shortwave radiation which penetrates (about 60%) can have a marked effect not only on the subsurface heat budget but also upon the potential biotic niches. The differentiation, between wavelength regions, of this fraction of solar radiation has been examined by e.g. Field and Effler (1983), Kirk (1983), Effler et al. (1984).

Each of the flux terms in equation 16 can be related to the meteorological (and astronomical) forcing parameters. Parameterization in terms of cloud cover, air temperature etc. have been sought over the last few centuries (e.g. Dalton 1802, Ångström 1924). A recent review of the wide selection of currently utilized parameterizations is given in Henderson-Sellers (1986).

MODELING THE EUTROPHICATION PROCESS

Modeling has now been accepted as an essential part of any lake restoration program. However, as no two waterbodies are alike, models often have to be adjusted to suit the local circumstances or may require substitution by a more appropriate model scheme.

Input-Output (Phosphorus) Models

Phosphorus models may be divided broadly into two classes: those which consider the lake as a blackbox and deal only with inputs, outputs and the total phosphorus mass in the lake; and those in which differential equations represent rates of change of phosphorus at different spatial locations and of different fractional forms. Each class may contain steady state models, seasonal models or annual models, models which include exchanges with the sediments, well-mixed models and multi-box models. The utility of each model depends upon the question to be answered together with a statement of uncertainty with which the model predictions are made. For example, for a lake which freezes in winter, annual variability in phosphorus loading becomes more marked, since phosphorus may be retained in the ice cover until it is released "quasi-instantaneously" at ice-melt in spring.

Input-output models are often based on the original work of Vollenweider (1968 1969). This model was the first to relate all the applicable parameters concerned in eutrophication, by assuming all nutrients to be well mixed. As with many, more sophisticated models its basis is the assumption of continuity (or mass balance), applied here to the net nutrient balance. Continuity is calculated both from nutrient inputs and outputs from the system associated with stream inflows and outflows, and from nutrients released (e.g. from sediments and decaying algae) into the water column. Based on data from only 20 lakes, he found a correlation between annual areal nutrient loading and the mean lake depth for a given trophic status. In this model it is assumed that:

- (1) the input phosphorus is immediately mixed throughout the lake (obviously inapplicable during the summer stratification, although on the annual timescale this limitation produces no immediate problems);
- (2) the outflow concentration is equal to the concentration prevailing in the lake;
- (3) the sedimentation rate of phosphorus is proportional to its concentration;
- (4) seasonal fluctuations in loading may be neglected. The model is thus most applicable for calculations of the steady state or year-to-year changes.

An alternative approach is to parameterize the mass balance equation in terms of an apparent settling velocity. In this approach, the deposition rate becomes a function of the bottom surface area. This model was used by Dillon and Rigler (1974) for oligotrophic and mesotrophic lakes in Southern Ontario. They found high correlations ($r \sim 0.85$) between predicted and actual phosphorus values.

Such models imply that the phosphorus concentration can be decreased by increasing the annual sedimentation rate (for example, using a sedimentation rate proportional to the square of the concentration) or the flushing rate, although the advantages of a higher flushing rate are partially negated by the accompanying decrease in the phosphorus retention coefficient.

Input-output models such as these are discussed in detail by e.g. Reckhow and Chapra (1983a). Vollenweider points out that the model neglects the possibility that there may be an internal phosphorus loading (from the sediments) and suggests that a modified model should be used in which the loading is plotted, not against mean depth, but against \bar{z}/t_w , where t_w is the mean residence time of the water (lake volume/yearly water discharge).

Although the solution sought is that of a criterion of trophic status for a lake of given annual phosphorus loading, mean depth and hydraulic residence time it should be noted that the trophic states are in effect a continuum from oligotrophy to eutrophy and, hence, the idea of associating a probability with each of the trophic states is to be recommended (OECD 1982). Defining a "critical" level, which may be needed as part of any water quality legislation, thus cannot be done easily. The concept of critical loading is thoroughly discussed by Vollenweider (1976) and a new model is developed to give L_{crit} in terms of the hydraulic load, $q_n = \bar{z}/t_w$

$$L_{crit} = 10q_n(1 + \sqrt{\bar{z}/q_n}). \quad [17]$$

Vollenweider's models of the input-output type appear reasonably well validated in terms of temperate zone lakes. However, to gain a wider use and acceptance, it is necessary to validate the models for lakes in other climatic regions, although preliminary results from Australia and South Africa have not been overconvincing (Smalls, p.c., 1988; Robarts, p.c., 1987).

Multi-Layer Models

To study seasonal variations it is necessary to formulate a model using at least two compartments - corresponding to the epilimnetic and hypolimnetic water masses (e.g. Imboden 1974). Two differential equations are formulated to describe the P fraction transformation rates. The model has two modes of operation - summer stagnation (2 layers) and winter circulation (1 layer). As with any temperature model which is similarly formulated, this is somewhat unrealistic, especially during the spring warming period. A similar, yet alternative, model stipulates a stratification period of exactly six months when the hypolimnion is assumed to remain oxic (a supposition not supported by many observations) and inputs of phosphorus from the sediments are neglected. Useful guidelines are given for utilization of such a model for management purposes. This model has been applied by the model developers to lakes with a wide range of detention times, who claim "excellent" results for their calculations of average phosphorus concentrations. However, application of the model by others to Lake Shagawa (Snodgrass and O'Melia 1975) underestimated the epilimnetic phosphorus concentrations.

In a modeling study (Bradford and Maiero 1978) of a proposed earthfill dam on the Delaware River near Tocks Island, New Jersey in respect of probable trophic state, two models were used - the two compartment model of Imboden (1974) and the input-output model of Dillon (1975). These modeling experiments suggested that 95% P removal should be implemented at the four

largest wastewater treatment plants in the area and that a significant amelioration could be achieved by decreasing non-point sources (especially agricultural) by 50%.

However a model containing only two layers (often of pre-specified depths), representing epilimnion and hypolimnion respectively must, de facto, only be applicable to a stratified situation as during summer. The period of the year when the lake is not stratified (approximately September/October until March/April) cannot be realistically simulated in this way. The justification for the use is that it is during the stratification period that the problems of algal blooms occur. However, for a more reliable model, which can predict phosphorus levels both throughout the year and from year-to-year, it is necessary to utilize multi-layer models, which incorporate the temporal development of thermal stratification. Consequently, one of the major lines of development has been that of multi-layer stratification models by the addition of chemical and biological species. Since these were originally developed by agencies with an engineering bias, they typically "lump together" the various identifiable biotic species into a smaller number of variables. For example, equations for DO and BOD were added to the one-dimensional Massachusetts Institute of Technology (MIT) thermal model (Markofsky and Harleman 1973). Assuming the surface to be saturated they proposed two alternative models: i) the entire euphotic zone is maintained at saturation by photosynthetic production and surface reaeration; and ii) the saturation exists to a smaller depth. Field tests in Fontana Reservoir were used to test the model's sensitivity to assumed values of inflowing BOD and BOD decay rate constant.

The Minnesota Lake Temperature Model (e.g. Stefan and Ford 1975) has been recently adapted to describe phosphorus cycling and phytoplankton blooms following a destratification event in Lake Calhoun (Gulliver and Stefan 1982). Homogeneity is maintained within the surface layer, sediment releases are specified as input and not calculated within the model, and the destratification is modeled on a simple vertical advection/entrainment of mass without consideration of feedbacks to turbulent diffusion alterations. The authors demonstrate that a large algal bloom follows the release of hypolimnetic nutrients upon the initiation of destratification, which would otherwise not have occurred (implying that the phytoplankton system was phosphorus limited). Reorientation of the model toward the calculation of turbidity in shallow lakes (Stefan et al. 1982, 1983), in which the model was renamed RESQUAL II, permitted simulations to be undertaken for Lake Chicot in Arkansas. The model does however possess a relatively large number of site-specific coefficients which must be calibrated separately for each new case study.

Work at the Waterways Experiment Station of the US Army Corps of Engineers has also concentrated on the development of dynamical models. Using two different assumptions regarding the parameterization of vertical mixing processes, they have developed two models for water quality simulation: WESTEX (Holland et al. 1982) and CE-QUAL-R1, the latter being the ecosystem extension of the thermal model CE-THERM. The model CE-QUAL-R1 (Environmental Laboratory 1982) contains 34 variables including nitrogen and phosphorus cycles, carbon cycling and several trophic levels in addition to the physical factors of CE-THERM, but, as noted above, requires tuning to a specific lake before use. It is a one-dimensional model intended to be appropriate only for the deepest part of the lake. Although originally developed from a strictly thermal model, it now has many of the attributes of the more biologically-orientated models, e.g., developed at Rennselaer Polytechnic Institute in New York State. Although the DO profiles are in reasonable agreement with observations, the other chemical parameters are not (Zimmerman 1984). This could perhaps reflect the problems of (i) incompatibility between the timescales necessitated by the model and the sampling interval; and (ii) the assumptions and simplifications made in developing the model, especially that of one-dimensionality.

Ecosystem And Eutrophication Models

At about the time that stratification-based models were being developed, groups with more biologically-oriented backgrounds were attacking the problem from their viewpoint. As their

emphasis has been on the accurate representation of the biochemical characteristics of an ecosystem (usually at the expense of the dynamics and thermodynamics), such models often with large numbers of "tuning coefficients", will be referred to collectively as ecosystem and eutrophication models (although some researchers differentiate between ecosystem models as placing more emphasis on detailed aspects of ecosystem dynamics than eutrophication models).

The calculations in ecosystem and eutrophication models are based on equations for mass balances. Kinetic formulations are needed for growth rates of phytoplankton etc., but it is not necessary to calculate growth for each individual species in the lake; indeed other sources and sinks may well be combined. Furthermore, many of the models do not try to predict the development of the thermal stratification but assume the epilimnion to be well mixed, restricting their analysis to times of the year when the lake can be assumed to be well represented by two static layers or by a single homogeneous layer (the "well-mixed reactor").

Experiments using an ecosystem model (Spraggs 1981) derived from the same source as the Waterways Experiments Station model CE-QUAL-R1 (see earlier discussion) initially produced a simulated DO depletion in the hypolimnion which was too rapid and suggested that this was due to an inclusion of both BOD and detritus as oxygen sinks. The BOD is a measure of the amount of dissolved organic material in the water column (and hence oxygen demand in its decomposition), whereas part of this material is also included in the detrital demand term. It is not possible to remove the detrital term since this recycles nutrients to the system. Similarly the BOD term is necessary to account for dissolved organics other than detrital decay and it is therefore recommended that both the BOD and detritus terms should be included, but the oxygen demand part of the detrital decay should be set equal to zero. This modified model was then tested and it was shown that DO concentrations in the bottom water were much more in accord with observations, the incorrect predictions of anoxia being remedied.

A large simulation model has been developed at Manhattan College in New York and utilized for Lakes Huron (Di Toro and Matystik 1977) and Erie (Di Toro and Connolly 1977). This model (which could almost be called an ecosystem model) utilizes fifteen variables. Versions of this model possessed initially only three layers (prespecified, not predicted), then seven layers, and hence straddle the divide between extended multi-layer models and comprehensive ecosystem models. The model contains a wide range of tunable parameters and has been shown to be useful in simulations of Lake Erie and Lake Ontario (e.g. Thomann et al. 1976). The calibrated results for chlorophyll- α , phosphorus and orthophosphorus show only fair agreement across the lake basin (although no statistical measures of goodness of fit are used; see model validation). However they do show the silica depletion in May, the nitrogen depletion in the western basin in July and the phosphorus depletion in the central and eastern basins in July, all of which can be connected with the termination of the two annual observed blooms. Additionally, this complex model is expensive in terms of computer time (Schnoor and O'Connor 1980). It has been suggested that realistic and useful results could be obtained by simplifying the system such that it is considered as well-mixed (realistic for impoundments of short detention time) or as a two-layer system (e.g., Imboden 1974). For the lake system, the steady-state solution is shown to be gained from a set of three equations. However there remain several rate constants to be determined in these equations - a disadvantage noted by the authors. Furthermore, the equations and the solution are found to provide a conceptual framework for the earlier work of Peter Dillon and co-workers with the addition of the phytoplankton to the predicted variables. The model has been applied to Lake Lyndon B. Johnson (the results being compared favorably with data from 1972 and 1973) (Schnoor and O'Connor 1980) and to Lake Ontario, a lake with a much higher retention time (with a reported similarly high level of success, following successful tuning).

The ecosystem model of Scavia et al. (1976a) has been applied successfully to several of the Great Lakes (Scavia et al. 1976b). In a further study (Scavia 1979), the model was used to examine the phytoplankton dynamics in Lake Ontario. The two-layer model includes parameterization of

available P, NH_3 , NO_x , dissolved N, soluble reactive Si, particulate Si, five groups of phytoplankton, six groups of zooplankton, the inorganic C system, sedimentary C, detrital C and benthic macroinvertebrates. This model has also been compared by Scavia and Chapra (1977) with the loading models of Dillon and others. The results are comparable under most circumstances. It is stressed that the choice of model should be determined by the temporal and spatial resolution required, balanced against the additional computational time that would be required to attain such resolution.

The ecosystem approach adopted at the Rennselaer Polytechnic Institute led to the development of the models CLEAN, CLEANER (developed for Lake George, USA but also applied to several European lakes) (Park et al. 1975) and then, after a modification to a multi-segment model, MS.CLEANER (Park et al. 1981) (including versions for use on mini- and microcomputers, e.g., Albanese et al. 1981). These models attempt to include a large number of variables, especially biological, which necessitated sacrificing some representativeness of the dynamic formulations. More recent versions incorporate more dynamical concepts and should therefore be more widely applicable without extensive recalibration. CLEANER utilizes the Steele (1965) light limitation function, nutrient limitation and full temperature dependence on all parameters. In addition, MS.CLEANER includes intracellular storage of nutrients and Michaelis-Menten kinetics, which is also formulated as a function of light and temperature. It has 40 state variables and provisions for horizontal and vertical transport. An application of MS.CLEANER to Övre Heimdalsvatn in Norway has also been undertaken with results for phytoplankton and zooplankton in relatively good agreement with observations.

As might be anticipated, the fine details of these large eutrophication models are beyond the scope of this review and the interested reader is encouraged to consult the original published papers and reports for further details. In addition, recent reviews appear in books on water quality modeling by Jørgensen (1980), Orlob (1983), Reckhow and Chapra (1983a) and Henderson-Sellers (1984). The fact that many of these ecosystem and eutrophication models are quite complex and characterized by a large number of parameters and state variables gives some cause for concern, which is discussed briefly in the next section.

MODEL VALIDATION

Verification and validation of water quality models are important, yet often neglected, components of any modeling study. Model construction and initial checking often utilizes a data set (often a year) for a specific lake or river. Verification and validation of the model, first for other years' data, then for other, totally unconnected, test sites gives the model developer and model user confidence that the model can be applied successfully - or, conversely, may indicate the limitations of applicability.

In all of the models discussed in this paper except the ADZ (section 2.2), rather informal methods of parameter tuning are normally utilized in calibration. More formal statistical methods of time-series analysis, such as those used in the ADZ modeling, are not normally considered, both because of the complexity of the models and the difficulty of obtaining appropriately large data sets which would allow for statistical identification and estimation. While this is justifiable in the circumstances, it should be realized that the lack of a formal statistical approach and the use of the more arbitrary parameter tuning can limit the credibility of the model (see Beck and van Straten 1983). Even when combined with sensitivity analyses and constraints on parameter values, such deterministic tuning is controlled, to some extent, by the modeler's prior prejudice and can be abused. In particular, the development of a model which reasonably matches a rather meager data set is no guarantee that the model is "valid" in wider terms, although it can still possess considerable practical utility.

Model acceptance, therefore, tends to rely on extensive testing, in which simulations and data are compared and evaluated for "correctness". In such comparative assessments, one of the greatest problems is that of subjectivity. There is, as yet, no agreed objective test for the quality of agreement between simulation and observation of most water quality models. Data are usually obtained as time series, representing space-and-time dependent values of the water quality variable under investigation. As such the data represent a stochastic description of the process - the data are realizations of random variables. In contrast, many of the water quality models discussed here are deterministic. The objective comparison of essentially random data and deterministically-derived simulation values is a current research goal for which the simple application of existing statistical tests for "goodness-of-fit" is inappropriate (Reckhow and Chapra 1983b, Beck and van Straten 1983, Young 1983, Henderson-Sellers, B. submitted for publication).

An alternative approach, which explicitly recognizes that models such as those discussed in the reservoir and the eutrophication processes will always be "speculative" to some degree, is the probabilistic simulation model proposed by Hornberger and Spear (1983) (see also Young, 1983) and used for the modeling of water quality in the Peel Inlet of Western Australia. Here, special Monte Carlo procedures are utilized to carry out a "generalized sensitivity analysis" which can lead either to the generation of hypotheses about the system behavior, or can be used to investigate different scenarios in the planning of management activities. Such models are not, however, considered to be "validated" in any sense, since no formal validation against data is attempted; and they cannot, therefore, be used for predictive purposes. Rather, they are simulation tests to extend the thought processes of the modeler within reasonable constraints.

One further problem is that the modeler and the manager responsible for one particular lake may have very different objectives dependent upon the use for which the water is to be put. Nevertheless a model simulation assessed as "excellent" should be able to be viewed as such from an objective viewpoint, regardless of the management objective function. It is almost certainly the case that judgement of simulations presented in the literature have an implicit bias towards accepting poor simulation in parameters of less concern. Parallel development of both models and quantitative assessment techniques is currently being undertaken by several authors.

OVERVIEW OF CURRENT MODEL DEVELOPMENT

In a state-of-the-art review of surface water quality modeling, checking what is currently being done in some of the major centers of model development seems to be indispensable. Consequently, a questionnaire was prepared (see Appendix 2) and sent to 30 centers, both in Europe and the U.S.A. This questionnaire was aimed primarily at identifying model developers and characterizing the models currently supported or under development, in order to find out some of the trends in model development. The mailing list was by no means exhaustive, given the short time available, but since the goal was not building an exhaustive model database (which would be a nice idea!) the answers represent a good subset, capable of elucidating some of the trends.

The 15 answers received were analyzed and the results summarized in table 1 found in Appendix 2. The careful analysis of these answer shows interesting results, presented in the following paragraphs.

Most models were initially developed using mainframes but the movement toward micros is evident for almost all the models reviewed, MS-DOS being the selected micro-environment, illustrating the effect that micros have had in the scientific community. The most widely used language is FORTRAN, although in one case a pre-processor including a simplified version of the model was written in PASCAL.

There is a clear distinction between well-established models and models that have been used solely by their developers. In fact it seems that most of the new models are developed in universities; but for a model to be widely used it needs a type of support that only research centers or planning agencies can give. The USEPA Water Quality Modeling Research Center (Barnwell et al. 1987) is a good example of that, having successfully maintained several models in the past ten years. Most developments, including updates and upgrades, are carried out by the universities, but user support is provided by the agency.

The most recent models, namely GELQAM (Straten et al. 1986), KWAL-NET and ADZ (Young and Ribeiro da Costa 1986) are rather complex models, with dynamic flows, inputs and processes, built to solve very specific problems requiring this type of model. Given the sparse responses, it is not possible to know if this corresponds to a clear trend or if the simpler models are not even reported. Stochastic models seem also to play a growing role, either as new models or upgrades to existing models. As an example, QUALII was extended to include a stochasticity in BOD and DO calculations using Monte Carlo techniques (Brown 1986).

Bringing some light into the ongoing discussion on lumped versus mechanistic model approaches, and classical Fickian versus other approaches, was one of the goals of this questionnaire. Most of the reviewed models are based on the Fickian dispersion equation, using either implicit or explicit finite difference solutions. Two of the models reviewed use different approaches: GELQAM uses a moving-cell plugflow with dispersion, and ADZ uses the ADZ equations. The questionnaires do not provide enough information to extend this discussion.

With regard to the range of variables simulated, the oxygen, nitrogen and phosphorus cycles seem to be quite well known processes, in which new developments are rare. Most innovative work is currently being done in toxic substance modeling.

Model output and post-processing is one of the areas in which the influence of the transition from mainframes to micros is more visible. Almost all the models on mainframes as batch jobs, with limited chance for the user to interfere with the ongoing processing. Much attention is being paid to develop interactive model post-processors, that either pick up a results file (frequently generated on a mainframe) and allow its interactive processing or show the results during the simulation, which is very rare.

Some of these post-processors have become rather sophisticated allowing, for instance, superposition of model results with real data obtained from a database and with thematic maps of the region being studied. QUALIII is a good example of this type of approach.

The idea of a model database mentioned above is already a reality. In fact some of the answers were received from the Bureau SAMWAT model database (Blumenthal et al. 1987). The flexibility and efficiency of this type of data base facilitate coping with the fast development that is taking place in this subject area all over the world.

CONCLUSIONS

Both for day-to-day water quality management and for longer-term planning exercises, mathematical models can provide a useful tool to supplement insights gained from both field and laboratory observations. Models of a wide range of complexity are becoming increasingly available for water quality studies and it is the selection, by the water quality manager, of the model most appropriate to a specific management goal that is perhaps one of the manager's greatest problems.

The research areas in river and stream water quality modeling which require immediate attention appear to be the comparison and more detailed analysis of the similarities and differences in the attributes of the ADE and the ADZ models for solute advection and dispersion in channels. Both model types have their merits and their relative practical utility will depend upon both the modeling objectives and the nature of the application.

The research areas in lake and reservoir water quality modeling which require immediate attention appear to be

- (1) the integration of continuously stirred reactor and process models for biological and chemical variables with higher resolution (temporal and spatial) physico-chemical (largely thermodynamic and hydrodynamic) 1-, 2- and 3-dimensional models;
- (2) the need to formulate better diffusion parameterizations for throughflows (especially for low retention time reservoirs and pumped storage reservoirs). At present, mass conservation is included but, in general, the mixing feedbacks between an underflow or interflow and the otherwise lentic water body itself are excluded.

As a final thought, mathematical modelers should be at least cognizant of (and hopefully will utilize) new mathematical theories, concepts and tools. In water quality modeling there has been little discussion of the potential use of catastrophe theory (but cf. Renguet and Dubois 1981) and the concept of chaos (Holden 1986). These tools are now available to the modeler - how can they best be used to improve both our understanding and ability to simulate reservoir ecosystems?

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APPENDIX 1: LIST OF SYMBOLS USED

A	cross-sectional area	$[L]^2$
\bar{c}	cross-sectional average solute concentration	$[M][L]^{-3}$
c_o	solute concentration at output of a single dead zone	$[M][L]^{-3}$
c_i	solute concentration at input of a single dead zone	$[M][L]^{-3}$
c_k	solute concentration at output of kth ADZ element	$[M][L]^{-3}$
c_{k-i}	solute concentration at previous (k-ith) ADZ element	$[M][L]^{-3}$
c_p	specific heat (at constant pressure)	$[L]^2[T]^{-2}[K]^{-1}$
D	the longitudinal dispersion coefficient	$[L]^2[T]^{-1}$
D_f	dispersive fraction (T_R/\bar{t})	dimensionless
f	Coriolis vector	$[T]^{-1}$
F	damping term in equation 13	$[M][L]^{-2}[T]^{-2}$
h	depth of mixed layer	$[L]$
k	decay rate coefficient	$[T]^{-1}$
K_H	coefficient of turbulent diffusion for heat	$[L]^2[T]^{-1}$
L_{crit}	critical phosphorus loading	$[M][L]^{-2}[T]^{-1}$
M	mass of solute	$[M]$
q_n	hydraulic load ($=\bar{z}/t_w$)	$[L][T]^{-1}$
Q_s	heat flux source term	$[M][L]^{-1}[T]^{-3}$
Q	discharge	$[L]^3[T]^{-1}$
t	time	$[T]$
\bar{t}	mean travel time of reach	$[T]$
t_w	mean residence time	$[T]$
T	temperature	$[K]$
T_R	ADZ Residence Time	$[T]$
\bar{u}	cross-sectional average longitudinal velocity	$[L][T]^{-1}$
v	vector velocity = (u,v,w); or (u,v) in two dimensions	$[L][T]^{-1}$
v_s	apparent settling velocity	$[L][T]^{-1}$
V	volume of single dead zone	$[L]^3$
V_e	ADZ volume	$[L]^3$
w_e	interfacial entrainment velocity	$[L][T]^{-1}$
x_i	spatial coordinates (x,y,z)	$[L]$
z	depth (measured vertically upwards or downwards from water surface - direction as specified in text)	$[L]$
\bar{z}	mean lake depth	$[L]$

Greek

α	ADZ parameters; equations 9, 11, 12	$[T]^{-1}$
α_H	molecular diffusivity of heat	$[L]^2[T]^{-1}$
β	ADZ parameters; equations 9, 11, 12	$[T]^{-1}$
ϵ	turbulent diffusion coefficients = ($\epsilon_x, \epsilon_y, \epsilon_z$)	$[L]^2[T]^{-1}$
ϕ_c	convective energy flux	$[M][T]^{-3}$
ϕ_e	evaporative energy flux	$[M][T]^{-3}$
ϕ_N	net energy flux at the air-water interface	$[M][T]^{-3}$
ϕ_{ri}	incoming longwave energy flux	$[M][T]^{-3}$
ϕ_{ro}	outgoing longwave energy flux	$[M][T]^{-3}$
ϕ_o	incoming shortwave energy flux	$[M][T]^{-3}$
ρ_o	reference density	$[M][L]^{-3}$
ρ_w	water density	$[M][L]^{-3}$
τ	time lag (ADZ advective time delay)	$[T]$

prime indicates perturbation quantities and overbar indicates mean value

APPENDIX 2

Questionnaire sent to model development centers

STATE - OF - THE - ART REVIEW

OF

SURFACE WATER QUALITY MODELS

(from the modelers perspective)

for the

INTERNATIONAL SYMPOSIUM ON WATER QUALITY MODELLING OF
AGRICULTURAL NON-POINT SOURCES
UTAH STATE UNIVERSITY
UTAH, June 1988

1 - MODEL IDENTIFICATION

MODEL NAME :

DEVELOPED INITIALLY BY : IN :

IMPLEMENTED ORIGINALLY IN : MAINFRAME ☐ ; MICROCOMPUTER ☐

AVAILABLE NOW IN MAINFRAME ☐ ; MS-DOS ☐ ; MAC ☐

2 - MODEL CHARACTERIZATION

TIME SCALE : STEADY-STATE ☐ ; QUASI-DYNAMIC ☐ ; DYNAMIC ☐ FLOW
INPUTS
PROCESSES

SPACE SCALE : ONE DIMENSIONAL ☐ ; X - Y ☐ ; X - Z ☐ ; 3 - D ☐

SOLUTION : ANALYTICAL ☐ ;

NUMERICAL FINITE - DIFFERENCE ☐ : EXPLICIT ☐ ;
IMPLICIT ☐ ;

NUMERICAL FINITE ELEMENTS ☐ ;

CHARACTERISTICS ☐ ;

OTHERS

VARIABLES SIMULATED : CBOD ☐ ; NBOD ☐ ; SOD ☐ ; DO ☐ ;
ON ☐ ; NH3 ☐ ; NO2 ☐ ; NO3 ☐ ; TN ☐ ;
TP ☐ ; TIP ☐ ; TOP ☐ ;

4 - MODEL OUTPUT

ECHO OF INPUT DATA ☐ ☐

INTERMEDIATE PRINTS : Error messages ☐ ☐ ; Intermediate values ☐ ☐ ;

others

TABLES : Concentration-time ☐ ☐ ; Concentration-space ☐ ☐ ;

TABLES: defined by the user ☐ ☐ ; fixed ☐ ☐

interval between tables : definable ☐ ☐ ; fixed ☐ ☐

GRAPHIC OUTPUT : INTERACTIVE ☐ ☐ ; BATCH ☐ ☐

PLOTS TIME-CONCENTRATION ☐ ☐

AS MANY AS DESIRED ☐ ☐ ; FIXED SIZE AND TYPE ☐ ☐ ; FREE FORMAT ☐ ☐

PLOTS SPACE-CONCENTRATION ☐ ☐

AS MANY AS DESIRED ☐ ☐ ; FIXED SIZE AND TYPE ☐ ☐ ; FREE FORMAT ☐ ☐

OBSERVED DATA CAN BE SUPER IMPOSED ☐ ☐ ; HOW

OTHER :

.....

STATISTICAL TREATMENT :

.....

.....

.....

.....

5 - MODEL USE

MODEL HAS BEEN USED BY : Research teams ☐ ; Planning agencies ☐ ;
 Government ☐ ; Others

MODEL RESULTS HAVE CURRENTLY (OR HAS) INFLUENCED REAL DECISIONS :

.....
 HOW ARE RECOMMENDATIONS BASED ON MODEL RESULTS ENFORCED OR USED ?

.....

HOW EASY IS THE MODEL TO USE Easy ☐ ; Moderate ☐ ; Difficult ☐
 HOW WELL IS THE MODEL SUPPORTED Well ☐ ; Moderate ☐ ; Poor ☐
 HOW GOOD IS DOCUMENTATION Good ☐ ; Moderate ☐ ; Poor ☐
 DID YOU DO CHANGES No ☐ ; Yes ☐
 HOW EASY ARE CHANGES TO MAKE Easy ☐ ; Moderate ☐ ; Difficult ☐

MODEL HAS BEEN USED FOR ...

-EVALUATION OF THE PROBLEM : Residuals input determination ☐
 Assessment of risk ☐ ; Specification of a range of feasible water
 quality/use objectives ☐

-EVALUATION OF ALTERNATIVE CONTROLS : Determination of effectiveness of
 alternatives ☐ ; Cost-benefit analysis ☐

-DECISION AND PROMULGATION OF CONTROL PROGRAM :
 Water quality standard setting ☐ ; Optimal control strategies ☐

-IMPLEMENTATION OF CONTROL PROGRAM : Waste load allocation ☐ ;
 Negotiation and issuance of discharge permits ☐ ; Monitoring of
 program ☐

-POST-AUDIT OF PROGRAM :

6 - DOCUMENTATION

PLEASE SEND AVAILABLE DOCUMENTATION both on the model and model application

Table 1.
Features of available models based on survey response.

General data	Model Name	WASP	WASTOX	QUAL2E	HSPF	EXAMS	GELQAM	POLTRA	TOXRIV
	Author	Di Toro, al	Connolly, al	WRE, Semcoq	Johanson, al	Burns et al	Straten et al	Simons, Lam	Lam et al
	Country	USA	USA	USA	USA	USA	Netherlands	Canada	Canada
	First Version	1982		1972	1984	1982			
	Last Version			1986					
	Developped in	Main	Main	Main	Main	Main	Main	Main	Micro
	Available	MS-DOS	MS-DOS	MS-DOS	MS-DOS	MS-DOS	In preparation		MS-DOS
	Language	Fortran	Fortran	Fortran	Fortran	Fortran			
Built upon									
Time scale	flow	dynamic	dynamic	steady		dynamic	dynamic	dynamic	dynamic
	inputs	dynamic	dynamic	steady		dynamic	dynamic	dynamic	dynamic
	processes	dynamic	dynamic	quasi-dynamic		dynamic	dynamic	dynamic	dynamic
Space scale	1 - D	compartment	compartment	yes	yes	compartment			X
	2 - D	compartment	compartment			compartment		X-Y	X-Z 3 layers
	3 - D	compartment	compartment			compartment			
Based on		dispersion eq.	dispersion eq.			dispersion eq.		dispersion eq.	
Processes		mechanistic	mechanistic	mechanistic	mechanistic	mechanistic	mech+lumped	mechanistic	mechanistic
Numerical	analytical								
	finite-difference	explicit	explicit	explicit	explicit	explicit		explicit	implicit
	finite element								
	characteristics						moving cell		
Flow simul.	accessory model	linknode mode			kinematic wave		supplied		
	Manning's			yes			externally		yes
	Depth-velocity			yes				yes	yes
Simulates	Oxygen cycle	4		4	4		3	2	2
	Nitrogen cycle	5		5	5		2		
	Phosphorus Cycle	6		6	6		7	6	
	Bacteria	2		1	1				
	Algae			1	1		Chlorophyl A		
	Plankton	2						phyto	
	Toxics		yes			organic		organic	yes
	Metals		yes						
	Food-chain		yes						
	Other								
Model Input	# parameters	variable	variable				10	2 - 10	2 - 3
	# constants	variable	variable				12	2 - 10	4 - 5
Model Output	Batch								
	Interactive	batch	batch	batch	batch	batch	batch	batch	interactive
	Echo Input data	yes	yes	yes	yes	yes	yes	yes	yes
	Error messages	yes	yes	yes	yes	yes	yes	yes	yes
	Tables	Output to	Output to	yes	yes	yes	yes	yes	yes
	Plots	GDP or Lotus	GDP or Lotus				yes	yes	yes
	Post-processor	yes - MVP							
	Statistical treat.	yes	none	yes					relative error
	Compare with real dat								yes
Model Use	Research teams	many	yes	yes	yes	yes	yes	yes	yes
	Planning Agencies	many		yes	yes	yes		yes	yes
	Government	many	yes	yes	yes	yes		yes	
	Consulting			yes	yes	yes	yes		
	Friendliness	moderate	moderate	good	moderate	moderate	difficult	moderate	good
	Support	moderate	moderate	good	moderate	moderate	moderate	moderate	moderate
	Documentation	reasonable	reasonable	good	good	reasonable	dutch	reasonable	reasonable
	Changes	reasonable	reasonable	easy	reasonable	reasonable	difficult	reasonable	reasonable
Used for	Risk assesment		yes				yes		
	allocate waste loads	yes	yes	yes	yes	yes	yes	yes	
	water quality obj.	yes	yes	yes	yes	yes	yes	yes	yes
	standard setting	yes	yes	yes	yes	yes		yes	yes
	cost-benefit analysis	yes	yes	yes	yes	yes			
	analyse alternatives	yes	yes	yes	yes	yes		yes	yes
	control strategies	yes	yes	yes	yes	yes		yes	yes
	monitoring	yes		yes				yes	yes
	negotiation	yes	yes	yes	yes	yes			
Model Impact	Influenced decisions	yes	yes	yes	yes	yes	yes		
Post-Audit		yes						Lake Erie	
Distributed		EPA		EPA	EPA	EPA	Rijhswaterst.		
Price				free	free	free	for use		
Source		R. Thomann	R. Thomann	T. Barnwell	T. Barnwell	T. Barnwell	G. Straten	D. Lam	
		T. Barnwell							
References									

Table 1 (continued).

General data	Model Name	SIMCAT	KWAL-NET	WODA	DELWAO	MODQUAL	QUALIII	ADZ
	Author	Warn	Liiklema et al	Soncini et al	Brinkman, al	Pagee et al	Costa et al	Costa, Young
	Country	UK	Netherlands	Italy	Netherlands	Netherlands	Portugal	Portugal+UK
	First Version		development		1985	1981	1987	1988
	Last Version				1987	1985	in development	in development
	Developed in	Main	Main	Micro	Main	Main	Main	Main
	Available		Part in Micro	MS-DOS	MS-DOS	MS-DOS		MS-DOS
	Language				Fortran	Fortran	Fortran	Fortran
Built upon						QUALII	QUALII	
Time scale	flow	steady	dynamic	steady		steady	steady	dynamic
	inputs	steady	dynamic	quasi-dynamic		steady	steady	dynamic
	processes	steady	dynamic	steady		quasi-dynamic	quasi-dynamic	dynamic
Space scale	1 - D		X	X		yes	yes	yes
	2 - D							
	3 - D							
Based on			dispersion eq.					ADZ
Processes		empir. + lump.	empir. + mech.	empirical		mechanistic	mechanistic	lump + mechan
Numerical sol	analytical	statistical						
	finite-difference		explicit			explicit	explicit	
	finite element							
	characteristics			characteristics				
Flow simul.	accessory model							yes
	Manning's					yes	yes	
	Depth-velocity			yes		yes	yes	
Simulates	Oxygen cycle	C800	4	2			4	3
	Nitrogen cycle	NH3	4				5	4
	Phosphorus Cycle		4				6	
	Bacteria						1	
	Algae		1				1	
	Plankton		phyto					
	Toxics							
	Metals							
	Food-chain							
	Other							
Model Input	# parameters			9				
	# constants							
Model Output	Batch						interactive	interactive
	Interactive	batch	batch	interactive				
	Echo input data	yes		yes			yes	yes
	Error messages	yes		yes			yes	yes
	Tables	via Micro	yes	yes			yes	yes
	Plots	via Micro	yes	yes			interactive	interactive
	Post-processor	in a Micro					interactive	interactive
	Statistical treat.			various				
	Compare with real dat				possible		data-base con.	data-base con.
Model Use	Research teams		yes	yes			yes	yes
	Planning Agencies	Water Author.		yes			yes	
	Government							
	Consulting							
	Friendliness	good	moderate	good	moderate	moderate	good	
	Support	poorly	poor	good		good(payed)	poor	
	Documentation	poor	poor	poor		good	poor	
	Changes	reasonable		difficult				
Used for	Risk assesment	yes						
	allocate waste loads	yes	yes				yes	
	water quality obj.	yes	yes				yes	
	standard setting	yes					yes	
	cost-benefit analysi	yes					yes	
	analyse alternatives	yes	yes	yes			yes	
	control strategies	yes					yes	
	monitoring	yes					yes	
	negotiation	yes					yes	
Model Impact	Influenced decisions	yes						
Post-Audit								
Distributed					Delft Labs	Delft Labs		
Price					not fixed	fixed		
Source		A. Warn			SAMWAT Bur.	SAMWAT Bur.		
References								

DISCUSSION OF PAPERS PRESENTED IN TECHNICAL SESSION 4, PART 1: SURFACE WATER MODELS FROM THE MODELER'S PERSPECTIVE

Rick Allen¹, Presiding
Jim Dougherty², Recorder

PAPERS DISCUSSED

Surface Water Quality Models: Modeler's Perspective by H.G. Stefan, R.B. Ambrose, Jr. and M.S. Dortch

Water Quality Models: Rivers and Reservoirs by B. Henderson-Sellers, P.C. Young and J. Ribeiro da Costa

SUMMARY

Much of the discussion centered on future improvements in surface water models. Most participants were interested in increasing the degree of complexity of the models so that natural processes could be simulated in greater detail.

The area of most interest was linking watershed and surface water quality models. The main barrier to this is the differences in time scales of interest in the two processes. Interpolation and/or integration of the relevant model outputs within linking subroutines would be a possible means of dealing with this difficulty.

Several other areas of improvement in model design were indicated. Groundwater/surface-water interactions were seen as being significant in some areas. This phenomenon is not commonly considered due to lack of information. An additional area of interest was the effect of sediment/water interactions on oxygen demand in some surface waters. The complex nature of this problem indicates much work would be required to adequately characterize the problem. The use of multilayered models was also seen as an area which should be given greater attention.

Some concern was voiced that too much effort was being expended in modeling the physical processes, when in many cases what is of interest is the biological response to these processes. Incorporation of the inherent uncertainties in predictions of biological processes should be of great concern in future modeling efforts.

The highly complex nature of biological systems should be studied in much greater detail. Much of this difficulty is due to the lack of communication between field researchers and modelers. The solution to this problem is to have modelers involved when field sampling is initially designed. This will insure that information necessary to both parties is collected. Information regarding the physical characteristics of the sample area, as well as biological composition, must be collected so that it will be of use to both groups. In absence of this information, adequate linking of biological and physical models will not be possible.

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A final area of concern was consideration of the accuracy of model predictions. The establishment of some type of confidence intervals for model output would allow comparison of different model predictions. In some cases, models which are less complex may provide better predictions than a more detailed model. Model applicability can be evaluated by the use of Monte-Carlo methods, sensitivity analysis and other methods. This would provide model users with a means to associate a level of confidence with the model predictions. These procedures are not generally available to most users and should be included in model development and modification.

